Modeling for Insight Using Tools for Energy Model Optimization and Analysis (Temoa)

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Abstract

This paper introduces Tools for Energy Model Optimization and Analysis (Temoa), an open source framework for conducting energy system analysis. The core component of Temoa is an energy economy optimization (EEO) model, which minimizes the system-wide cost of energy supply by optimizing the deployment and utilization of energy technologies over a user-specified time horizon. The design of Temoa is intended to fill a unique niche within the energy modeling landscape by addressing two critical shortcomings associated with existing models: an inability to perform third party verification of published model results and the difficulty of conducting uncertainty analysis with large, complex models. Temoa leverages a modern revision control system to publicly archive model source code and data, which ensures repeatability of all published modeling work. From its initial conceptualization, Temoa was also designed for operation within a high performance computing environment to enable rigorous uncertainty analysis. We present the algebraic formulation of Temoa and conduct a verification exercise by implementing a simple test system in both Temoa and MARKAL, a widely used commercial model of the same type. In addition, a stochastic optimization of the test system is presented as a proof-of-concept application of uncertainty analysis using the Temoa framework.

Keywords: energy economy, open source, repeatability, uncertainty analysis, stochastic optimization

1. Introduction

With multi-decadal time horizons and geographic scales ranging from local (Bhatt et al., 2010; Morris et al., 1996) to global (Weyant, 1993), energy economy optimization (EEO) models have emerged as critical tools for the assessment of energy technology and public policy. However, the prevailing approach to model development and application limits the insight that can be drawn from modeling applications, as outlined in Figure 8. In developed countries – particularly the U.S. and Western European nations – Moore's Law coupled with the increasing availability of energy, economic, and environmental data have catalyzed the development of increasingly complex EEO models. In addition, multi-decadal timescales for analysis prevent the timely comparison of model projections to real world outcomes, so the steady growth in model complexity remains unchecked by robust model validation exercises. Models are further obfuscated by a general lack of publicly available source code and data (DeCarolis et al., 2012). As a result, the application of complex, opaque models leads to two negative outcomes: (1) an inability for third parties to verify model results and (2) difficulty in performing uncertainty analysis.

Because EEO models necessarily have long future timeframes, expansive system boundaries, and encompass both physical and social phenomena, the level of descriptive detail provided in model documentation and

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peer-reviewed journals is insufficient to reproduce a specific set of published results. More generally, the precise replication of results with computational models requires access to source code and data (Ince et al., 2012; Hanson et al., 2011; Barnes, 2010).

Large, complex models are also computationally expensive and therefore difficult to iterate, which deters efforts to perform sensitivity and uncertainty analysis. As a result, treatment of uncertainty in EEO model-based analysis is often limited (e.g., EIA, 2012; Clarke et al., 2007; Nakićenović et al., 2000; IEA, 2010). Complex models are often used to produce a small number of illustrative scenarios that contribute relatively little insight about the system under consideration (Morgan and Henrion, 1990). The focus on a limited set of highly detailed scenarios can also produce cognitively compelling storylines that lead to systematic overconfidence in the results presented (Morgan and Keith, 2008). The poor performance associated with past efforts to predict future energy outcomes supports this assertion (Craig et al., 2002).

This paper introduces Tools for Energy Model Optimization and Analysis (Temoa), an open source modeling framework used to conduct energy system analysis with a technology explicit energy economy optimization (EEO) model. We aim to address the issues of verification and uncertainty quantification by (1) instituting a transparent process for EEO model development and application that facilitates independent third party verification, and (2) implementing rigorous uncertainty analysis in a high performance computing (HPC) environment. Section 2 outlines our long term goals and justification for creating Temoa. Section 3 describes how Temoa will meet our stated objectives. Section 4 gives an overview of the model's algebraic formulation, and Section 5 describes the software used to implement the Temoa formulation. Section 6 presents a verification exercise based on careful comparison to a simple MARKAL dataset. Section 7 presents a proof-of-concept application of stochastic optimization to illustrate the capability of the Temoa framework to conduct uncertainty analysis, and Section 8 draws conclusions and outlines future work.

2. Motivation

Energy model design should be driven by a clearly articulated research goal. Our long-term goal is to derive policy-relevant insight related to the cost, emissions, deployment, and coordinated operation of energy technologies over time while rigorously accounting for large future uncertainties. While simple and transparent accounting frameworks can be utilized to conduct such analysis, the specification of detailed, self-consistent assumptions across the energy system can be difficult and time consuming. By contrast, optimization models employ formal search techniques, which enable a rapid and systematic exploration of the decision space to identify solutions that meet a specified objective. We chose to build a technology explicit EEO model, which enables a simultaneously broad and deep assessment of technology by considering the economic and technical characteristics of individual technologies as well as their interactions within a well-defined system.

Prior to building Temoa, we conducted an extensive review of existing energy models (DeCarolis et al., 2012). Through a formal review of the International Energy Workshop annals over the last decade, we found that three-fourths of surveyed models do not provide access to model source code and data. Among those that do, OSeMOSYS (Howells et al., 2011) is closest in structure and function to Temoa but serves a complementary purpose. A key motivation for OSeMOSYS is to make energy system modeling accessible to a much broader community, including students and researchers in developing countries who often lack the time and financial resources required to utilize larger commercial models. While the Temoa project shares these goals by utilizing free software, its design was driven primarily by the desire to enable repeatability and perform uncertainty analysis. We believe that there is value in having more than one open source EEO model of the same type available to the energy modeling community, since two distinct models are never identical: the process of distilling the relevant literature into a mathematical model requires reasoned judgment that makes modeling as much art as science (Morrison and Morgan, 1999; Ravetz, 2003).

In addition to reviewing the process of EEO model development and application, DeCarolis et al. (2012) also investigated the broader field of scientific computing and used it to develop a set of recommendations that can help enable the replication of model-based results by third parties. The recommendations include making source code and input data publicly accessible, making transparency a design goal, and utilizing free software tools. We have implemented these recommendations in the design of the Temoa framework.

3. The Temoa Framework

The Temoa framework is designed such that the resultant model-based analysis is repeatable by third parties and provides an assessment of uncertainty that can affect outcomes of interest. We describe in Section 3.1 – Section 3.3 how these design objectives were met.

3.1. Transparency

To inform our approach to model transparency, we investigated the software engineering practices employed by three large scale scientific software projects: MPICH2, a high performance parallel programming library (Balaji et al., 2011); the Portable, Extensible Toolkit for Scientific Computation (PETSc), a parallel differential equations solver library (Balay et al., 2011); and the Community Earth System Model (CESM), a fully-coupled, global climate model (UCAR, 2013). Based on careful review of these projects, the Temoa framework has been designed to include the following features: (1) a public, web-enabled interface to model source code and data, (2) developer documentation to encourage community contributions, (3) an avenue for user and developer interaction, and (4) a software utility to visualize output.

3.1.1. Revision Control

The Temoa project provides public, web-enabled access to a revision control system (RCS), which provides the means to digitally store a complete archive of code changes (i.e., "commit" or "change" histories). Best practices suggest that the developer summarizes each commit to the repository. The resultant electronic archive enables structured development and provides an audit trail that enhances transparency for both Temoa developers and users.

A project may organize an RCS in a number of ways. One common approach divides the repository into a trunk and development branches, with the trunk representing the latest version, and the individual branches representing stable versions or experiments. Temoa's repository structure includes parallel development branches (and no trunk) with each branch tuned to explore a specific set of questions. In many cases, where additional functionality requires extensive modification to an existing model formulation, the existing version can remain distinct and be archived separately. By archiving different branches of Temoa, we intend to prevent creep in model complexity over time as a model is adapted to answer new questions. Our approach contrasts with OSeMOSYS, which is based on the development of separable component blocks that can be added or removed to a core version of the model to customize model functionality (Howells et al., 2011). Both approaches have strengths, but neither is perfect: it may be difficult to separate OSeMOSYS functionality into distinct component blocks, but it may also be difficult to integrate changes across different versions and branches of Temoa.

3.1.2. Documentation

While public access to code and data enables interested parties to interrogate the model, it will remain largely opaque in the absence of well-designed user documentation. We have implemented auto-generated documentation that fuses comment blocks in the source code with a clear narrative description. As described in Section 5, the Temoa model has been implemented in Python (Lutz, 2009). Python stores object comments in a special member variable, allowing third party tools to dynamically introspect a code base to generate documentation accessible to end users. In Temoa, comments interspersed in the source code contain LaTeX (Lamport, 1986) formatted algebraic formulations of associated equations that are automatically queried and combined with a separate descriptive narrative to dynamically create end-user documentation. The latest documentation is available on the project website (Hunter et al., 2013). This streamlines the documentation effort by allowing developers to focus on embedding descriptive comments in the source code, which also eliminates discrepancies that arise from maintaining multiple forms of documentation.

3.1.3. Communication and Interaction

A successful open source model must provide a means for users and developers to interact. The developers of PETSc and MPICH2 are highly responsive to user queries on their traffic-intensive mailing lists (MPICH2, 2013; PETSc, 2012). While currently we do not have the same traffic as these well-established projects, we use an online forum for communication among developers as well as interaction with end users.

3.1.4. Visualization

Both PETSc and CESM include visualization tools to help users interrogate model behavior. In our case, model accessibility and transparency relies in part on the capability to visualize the energy system network under consideration. To meet this need, we employ an open source graphics package called Graphviz (Ellson et al., 2002) to dynamically generate an energy system map at model runtime. The Graphviz layout programs take descriptions of graphs in a simple text language, and create diagrams in several formats. Graphviz operates on a text file produced at model runtime that describes the nodes and edges within a given graph. Figure 8 provides an illustrative energy system map. Temoa also generates a set of navigable output graphics by model time period that superimpose the resultant commodity flows and technology capacities on the graph. In addition to the output graphic, the Graphviz text input provides an auditable model record that can be used for debugging and verification purposes.

3.2. Replication of Model Results

The RCS serves another important objective: to archive "snapshots" of source code and data used to produce published model analysis. To our knowledge, Temoa is the first EEO modeling effort to provide public access to a revision control system, which enables third parties to precisely replicate our published results by accessing archived versions of source code and data. While other open source models such as OSeMOSYS (Howells et al., 2011), AIM (Kainuma et al., 1998), and DICE (Nordhaus, 1993) exist, none publicly archive source code and data in a consistent manner that enables precise replication of published results by third parties.

3.3. Uncertainty Analysis

A key challenge associated with energy modeling is to derive actionable insight in the face of large future uncertainties. Many prior efforts have made future uncertainty the focus of model-based analysis (Kanudia and Loulou, 1998; Gritsevskyi and Nakićenovi, 2000; Labriet et al., 2008). From its initial conceptualization, Temoa was designed for operation in a multi-core, multi-node compute environment, which significantly expands the capability to perform sensitivity and uncertainty analysis. We do not intend to use the enhanced computational ability to solve large and complex datasets. Rather, our intention is to build datasets that are only as detailed as needed to meet the research objective at hand, and to focus effort on iterating the model to understand how key uncertainties can drive the model results.

Model uncertainties can arise from two sources: the imprecise specification of input data (parametric uncertainty) and the limited ability of model equations to represent reality (structural uncertainty). Parametric uncertainty can be addressed in a variety of ways: scenario analysis to quantify how exogenous drivers affect model outputs, sensitivity analysis to identify the input parameters that produce the largest effect on model outputs, and uncertainty analysis via Monte Carlo simulation to provide a measure of dispersion in the outputs. Running an energy model in an HPC environment facilitates sensitivity and uncertainty analysis by enabling the simultaneous execution of multiple model runs across available compute cores.

Because each model realization produced with one of the techniques above assumes (a priori) a particular state of the world based on the input values drawn, the parameter uncertainty is propagated through the model. Resolution of uncertainty before the optimization is performed represents a "learn then act" approach (Kann and Weyant, 2000). Such an approach is of limited utility to a decision maker, who must make decisions in the face of uncertainty by taking an "act then learn" approach. Multi-stage stochastic optimization embeds the probability of different outcomes within the model formulation via specification of an event tree, yielding a near term hedging strategy that accounts for future uncertainties (Loulou and Lehtila, 2007). Such hedging strategies provide insight relevant to policy makers, investors, and planners, who must make decisions before uncertainty is resolved (Holthausen, 1979). The complexity of event trees is often limited by the computational difficulty in solving the extensive form of the problem specification with classical solution methods. While stochastic optimization has been applied to energy system models, the model complexity and computational requirements have limited analysis to relatively simple probability trees. For example, Kanudia and Loulou (1998) implemented 8 scenarios across 3 time stages, Loulou and Kanudia (1999) implemented 5 scenarios across 2 time stages, Labriet et al. (2008) implemented 8 scenarios

across 2 time stages, Bosetti and Tavoni (2009) implemented 3 scenarios across two stages, and Babonneau et al. (2012) implemented 4 scenarios across 2 time stages. The implementation of the Temoa framework on a compute cluster using solution algorithms that involve the use of distributed memory, such as progressive hedging (Watson and Woodruff, 2010), allow the specification of event trees that are more complex, thereby enabling us to address future uncertainty in a more comprehensive manner. Section 7 discusses a stochastic optimization of a simple model with 81 scenarios across 3 time stages, and we have solved internal test formulations with 512 scenarios across 4 time stages (albeit with a simple energy system representation).

All of the techniques discussed thus far address parametric uncertainty. Given the limited ability of EEO models to represent real world energy markets, structural uncertainty is a critical consideration. In future work, we plan to address the structural uncertainty in the Temoa model formulation through the application of modeling-to-generate alternatives, which provides a way to systematically search the model's near optimal decision space for alternative solutions that account for unmodeled objectives (DeCarolis, 2011).

4. Model Formulation

The core component of the Temoa framework is a technology explicit energy system model. The model objective is to minimize the present cost of energy supply by deploying and utilizing energy processes and commodities over time to meet a set of exogenously specified end-use demands. The energy system is described algebraically as a network of linked processes that convert raw energy commodities (e.g., coal, oil, biomass, uranium, sunlight) into end-use demands (e.g., lighting, transport, water heating) through a series of one or more intermediate energy forms (e.g., electricity, gasoline, ethanol). Each process is defined by a set of engineering, economic, and environmental characteristics (e.g., capital cost, efficiency, capacity factor, emissions rate) associated with converting an energy commodity from one form to another. Processes are linked together in a network via model constraints representing the allowable flow of energy commodities.

Technology explicit models are typically formulated as linear programming problems in which continuous amounts of technology capacity are utilized to meet end-use demands. In cases where non-linear relationships exist, such as supply curves for raw energy commodities, a piecewise linear approach can be taken (Loulou et al., 2004). The Temoa model formulation is similar to the MARKAL/TIMES model generators (Fishbone and Abilock, 1981; Loulou et al., 2005), MESSAGE (Messner and Strubegger, 1995), and OSeMOSYS (Howells et al., 2011).

4.1. Treatment of Time

The Temoa model optimizes energy system infrastructure and performance across several timescales. The longest scale is the complete set of periods (P) considered by the model, which is in turn divided into two distinct sets: 'existing' (P^e) , and 'future' (P^f) . The existing time set defines the technology capacity vintages that exist prior to the periods in the future time set, and the model will return results for the periods in the future time set.

Both time sets $(P^e \text{ and } P^f)$ consist of user-defined periods, which represent an aggregation of the years from one period to the next. For example, if the first three time periods in a Temoa model are 2010, 2015, and 2025, then the 2010 time period represents the years 2010 through 2014, and the 2015 time period represents the years 2015 through 2024. Note that the length of each period is determined dynamically from the time between adjacent periods in P^f , allowing (for example) the user to specify shorter periods near the present and longer periods into the future when uncertainty is larger. Within each period, Temoa performs the optimization for a single characteristic year, with all capacity and activity results assumed to remain the same for every year within the period. As such, the optimal results for each period correspond to a representative year within that period.

To capture the seasonal and diurnal variations in end-use demand and required technology capacity, each future year is divided into sets of seasons and times of day. Combinations of each season and time of day form time slices (e.g., winter-day, summer-night). The formulation in Sections 4.2 - 4.6 describes how Temoa optimizes technology capacity and utilization across these time units.

4.2. Introduction to Model Algebra

Algebraic models generally consist of four distinct components: sets, parameters, variables, and equations. A set is a collection of user-specified elements used by the model to index parameters and variables. For example, Temoa contains a set T that represents the set of all technologies considered by the model. The user must define the elements of T (e.g., pulverized_coal, wind, electric_car), which Temoa uses to index various parameters and variables. For instance, the investment cost $IC_{t,v}$ is indexed by $t \in T$ and $v \in V$ such that each defined vintage of each technology is assigned an investment cost.

Table 1 explains the nomenclature in Temoa's formulation. There are a total of 6 unique sets as well as several subsets and alias sets. Capital subscripts represent the set names and lower case subscripts represent individual set elements (e.g., $c \in C$). Note that all commodities (c) belong to the set C, but for notational clarity in the formulation, we define aliases for individual set elements to represent input commodities ($i \in C$) and output commodities ($o \in C$). Note also that because most parameters, variables, and constraints are sparsely indexed, Θ denotes the sparse superset representing the valid combinations of individual set elements. The subscript to Θ denotes a specific sparse superset, which can be identified by context. For example, the Demand constraint class (eq. 3) is only useful for the specific indices of the end-use demand and demand-specific distribution parameters (p, s, d, and c) that are specified by the modeler in the associated data file. We denote this sparse subset of valid indices by Θ_{demand} .

The ordering of the set indices is consistent throughout the model to promote an intuitive "left-to-right" description of each parameter, variable, and constraint set. For example, Temoa's output commodity flow variable $\mathbf{FO}_{p,s,d,i,t,v,o}$ can be described as follows: "in period (p) during season (s) at time of day (d), the flow of input commodity (i) to technology (t) of vintage (v) generates an output commodity flow (o) of FO." While not all variables and parameters are indexed by all the sets shown above, they all follow the same left-to-right ordering scheme. In this manner, for any indexed parameter or variable within Temoa, a left-to-right, arrow-box-arrow describes the input \rightarrow process \rightarrow output flow of energy. A visual depiction of the commodity flow into and out of a given process is provided in Figure 8.

A key parameter is technology efficiency $EFF_{i,t,v,o}$, which defines the output (o) per unit input (i) of each process $\langle t, v \rangle$. Temoa uses the modeler-specified indices of the EFF parameter to build the sparse Θ superset of valid indices for every other parameter, variable, and constraint.

4.3. Decision Variables

The lowest level decision variable in the model is the commodity flow out of a technology (**FO**). The technology- and vintage-specific activity and capacity are in turn derived from **FO**. In Temoa, the total commodity production from a process is referred to as its "activity":

Process Activity:

$$\mathbf{ACT}_{p,s,d,t,v} = \sum_{i,o} \mathbf{FO}_{p,s,d,i,t,v,o} \tag{1}$$

$$\forall \{p, s, d, t, v\} \in \Theta_{\text{activity}}$$

Since the activity variable (**ACT**) is given by the sum over the commodity inputs and outputs associated with the output flow variable **FO**, a technology's activity level is always measured by its commodity production rather than consumption. The summation over both i and o is required to accommodate a many-to-one or many-to-many input-output commodity mapping. The **ACT** variable in turn determines the required technology capacity (**CAP**):

Technology Capacity:

$$(CF_{s,d,t,v} \cdot C2A_t \cdot SEG_{s,d} \cdot TLF_{p,t,v}) \cdot \mathbf{CAP}_{t,v} \ge \mathbf{ACT}_{p,s,d,t,v}$$
(2)

$$\forall \{p, s, d, t, v\} \in \Theta_{\text{activity}}$$

The capacity factor (CF) represents the maximum availability of a process by season and time-of-day, as determined by resource availability (e.g., as with intermittent renewables) as well as forced and unforced outage rates. The segment (SEG) is critical because the required amount of technology-specific capacity depends on the period of time over which the production occurs. For processes whose lifetimes end within period p, Equation (2) limits the activity by the scaling factor TLF. The user is responsible for ensuring the consistency among units through the proper specification of C2A. While the CAP variable relates to ACT via an inequality constraint, the constraint will remain binding where new capacity has a positive cost. Equation (2) also applies to preexisting capacity, where the variable CAP is replaced by the parameter ECAP.

4.4. Physical and Operational Constraints

There are several constraints required to represent the critical physical and operational requirements associated with an energy system. The requirement that supply is sufficient to meet demand drives all other constraints: the model must ensure that the exogenously specified annual end-use demands $(DEM_{p,c})$ – distributed per slice according to the demand-specific distribution $(DSD_{s,d,c})$ – are satisfied by the available commodity output:

Supply-Demand Constraint:

$$\sum_{i,t,v} \mathbf{FO}_{p,s,d,i,t,v,c} \ge DEM_{p,c} \cdot DSD_{s,d,c}$$
(3)

$$\forall \{p, s, d, c \in C^d\} \in \Theta_{\text{demand}}$$

While Equation (3) requires commodity production to meet an end-use demand, it does not specify how the end-use commodities are produced. A constraint is needed to determine how commodity inputs and outputs relate at the individual process level:

Process-Level Commodity Flow Constraint:

$$\mathbf{FO}_{p,s,d,i,t,v,o} \le EFF_{i,t,v,o} \cdot \mathbf{FI}_{p,s,d,i,t,v,o} \tag{4}$$

$$\forall \{p,s,d,i,t \in T - T^s, v, o\} \in \Theta_{\mathrm{flow}}$$

Equation (4) ensures that the commodity output of a process cannot exceed the product of the commodity input and efficiency, enforcing conservation of energy at the process level. In addition, indexing efficiency by both input and output commodities provides a flexible technology characterization capable of tracking multiple commodity flows into and out of a single technology. For example, a flex fuel vehicle can consume an ethanol blend or gasoline to produce vehicle miles traveled, each with different efficiencies. (Note that $T - T^s$ indicates the subset of T that does not include T^s . Thus, Equation (4) applies to all non-storage processes.) Equations (3) and (4) ensure that demand is met by a demand technology, but an additional constraint is needed to connect the inputs to demand technologies with upstream outputs:

Global Commodity Balance Constraint:

$$\sum_{i,t,v} \mathbf{FO}_{p,s,d,i,t,v,\mathbf{c}} \ge \sum_{t,v,o} \mathbf{FI}_{p,s,d,\mathbf{c},t,v,o}$$
(5)

$$\forall \{p, s, d, c\} \in \Theta_{\text{balance}}$$

Note that Equation (5) sums over all technologies and all vintages that produce or consume commodity c (in bold to make clear the placement of indices as input and output). For each period p, season s, time of day d, and commodity c, the left and right sides represent the total commodity produced and consumed, respectively. Taken together, Equations (3), (4), and (5) create a network that links technologies together via allowable flows of energy commodities, thereby defining a set of feasible energy pathways that map raw resources to end-use demands.

According to Equation (5), outputs from technologies producing intermediate commodities are optimized for each season and time of day combination (i.e., at the "time slice" level). This is desirable for electric generators, for example, which are dispatched to meet demand within each time slice based on the delivered cost of energy. Equation (5) does not apply to demand devices, however, which are not shared resources like electric generators. Instead, the utilization of each demand device type must remain proportional in each time slice. For example, electric heater activity should not be optimized by time slice because the end-users utilizing the capacity rely on it in each time slice with a heating demand. The following constraint ensures proportional production in each time slice for all demand devices:

Demand Activity Constraint:

$$DSD_{s,d,c} \cdot \sum_{i} \mathbf{FO}_{p,s',d',i,t,v,c} = DSD_{s',d',c} \cdot \sum_{i} \mathbf{FO}_{p,s,d,i,t,v,c}$$

$$\tag{6}$$

$$\forall \{p, s, d, t, v, c \in C^d, s' \in S - \{s\}, d' \in D - \{d\}\} \in \Theta_{DemandActivity}$$

Similar to Equation (4), the notation in Equation (6) for d' indicates that the set element d' belongs to the set D but cannot take on the value d, denoted by $\{d\}$. (The same interpretation applies to s'.)

Two additional constraints relate specifically to electric generators. First, due to their thermal properties, baseload plants cannot shift output over the course of a day to follow load. As a result, all technologies in the baseload subset (T^b) must produce the same activity per unit time in each time-of-day segment, but can vary their output rate across seasons:

Baseload Constraint:

$$SEG_{s,d'} \cdot \mathbf{ACT}_{p,s,d,t,v} = SEG_{s,d} \cdot \mathbf{ACT}_{p,s,d',t,v}$$
(7)

$$\forall \{p,s,d,t \in T^b, v, d' \in D - \{d\}\} \in \Theta_{\mathrm{baseload}}$$

Second, a constraint is required to model energy storage. Technologies belonging to the T^s set are not subject to Equation (4), which requires that commodities in and out of a process be balanced within each time slice. Instead, storage technologies must balance input and output over the course of a season:

Storage Constraint:

$$\sum_{d} \left(EFF_{i,t,v,o} \cdot \mathbf{FI}_{p,s,d,i,t,v,o} - \mathbf{FO}_{p,s,d,i,t,v,o} \right) = 0$$
(8)

$$\forall \{p, s, i, t \in T^s, v, o\} \in \Theta_{\text{storage}}$$

4.5. User-Defined Constraints

The constraints provided in this section are not required to define proper system operation, but allow the modeler to specify additional limits to technology and commodity production. With regard to the utilization of natural resources, Temoa includes a constraint that limits resource consumption by a resource technology (i.e., domestic production or import) to a user-specified upper limit each period:

Resource Production Constraint:

$$\sum_{s,d,i,t\in T^r,v} \mathbf{FO}_{p,s,d,i,t,v,c} \le RSC_{p,c}$$
(9)

$$\forall \{p,c\} \in \Theta_{\text{resource}}$$

In addition, users may impose an upper or lower bound on the installed capacity of a specific technology each period:

Capacity Limits:

$$\mathbf{CAPAVL}_{p,t} \le MAX_{p,t} \qquad \forall \{p,t\} \in \Theta_{\max}$$

$$\mathbf{CAPAVL}_{p,t} \ge MIN_{p,t} \qquad \forall \{p,t\} \in \Theta_{\min}$$
(10)

$$CAPAVL_{p,t} \ge MIN_{p,t}$$
 $\forall \{p,t\} \in \Theta_{\min}$ (11)

CAPAVL is a summation of all active vintages of technology t, taking into account those processes whose lifetime ends prior to the end of period p.

For technologies with multiple outputs, it is often necessary to constrain the relative share of outputs to a user-specified fraction. Equation (12) allows a modeler to specify fixed proportions for multiple outputs from a single technology:

Technology Output Split Constraint:

$$SPL_{i,t,o} \cdot \mathbf{FO}_{p,s,d,i,t,v,o'} = SPL_{i,t,o'} \cdot \mathbf{FO}_{p,s,d,i,t,v,o}$$
 (12)

$$\forall \{p, s, d, i, t, v, o, o' \in C - \{o\}\} \in \Theta_{\text{split}}$$

Finally, users can track emissions by specifying an upper bound on emissions each period:

Emission Limit Constraint:

$$\sum_{s,d,i,t,v,o} \left(EAC_{e,i,t,v,o} \cdot \mathbf{FO}_{p,s,d,i,t,v,o} \right) \le ELM_{p,e}$$
(13)

$$\forall \{p, e \in C^e\} \in \Theta_{\text{emission}}$$

Though there are additional internal constraints to track reporting variables within the Temoa source code, the 13 constraint classes presented above, along with the objective function, represent the core model formulation.

4.6. Objective Function

Temoa minimizes the present cost of energy supply to meet the specified end-use demands. The scalar objective function value represents a summation of the capital, fixed, and variable costs related to the installation and utilization of all energy technologies:

$$Minimize$$
: TotalCost = LoanCost + FixedCost + VariableCost (14)

LoanCost, FixedCost, and VariableCost in Equation (14) represent the scalar sum of more detailed calculations presented in Equations (15), (16), and (17). LoanCost and FixedCost depend on the CAP variables and VariableCost depends on the **ACT** variables, which are both derived from **FO**. LoanCost represents the total amount paid on loans for capital investment:

$$LoanCost = \sum_{t,v} \left(\left[IC_{t,v} \cdot LA_{t,v} \cdot \sum_{y=0}^{MLL_{t,v}} \frac{1}{(1 + GDR)^{y+v-P_0}} \right] \cdot \mathbf{CAP}_{t,v} \right)$$
(15)

The inner sum calculates the appropriate discount factor associated with future loan costs for each technology vintage. P_0 denotes the first model year within P^f , so costs are discounted to the beginning of the first future period. The parameter MLL contains only natural numbers, and is the smaller of two quantities: the year the loan reaches maturity or the last year in P^f . The outer sum calculates the total loan costs associated will all technology vintages installed over the future horizon. Via the $LA_{t,v}$ parameter (representing the annuity on a capital investment¹), the user may represent technology-specific financing options.

The second term in Equation (14), FixedCost, represents annually recurring fixed costs:

$$\text{FixedCost} = \sum_{p,t,v} \left(\left[FC_{p,t,v} \cdot \sum_{y=0}^{MTL_{p,t,v}} \frac{1}{(1 + GDR)^{y+p-P_0}} \right] \cdot \mathbf{CAP}_{t,v} \right)$$
(16)

Equation (16) is similar to equation (15) and represents a present value calculation of all fixed costs but with different constants: the period- and process-specific fixed cost parameter (FC) replaces the process investment cost parameter (IC) and the process lifetime parameter (MTL) replaces the process loan lifetime parameter (MLL). Since there is no loan, there is no need for the loan annualization parameter (LA). Finally, the last term in Equation (14), VariableCost, represents the recurring variable costs:

$$VariableCost = \sum_{p,s,d,t,v} \left(\left[VC_{p,t,v} \cdot \sum_{y=0}^{LEN_p} \frac{1}{(1+GDR)^{y+p-P_0}} \right] \cdot \mathbf{ACT}_{p,s,d,t,v} \right)$$
(17)

For resource technologies that produce raw commodities such as petroleum and natural gas, VC represents the commodity extraction cost; for technologies that consume commodities, VC typically represents the variable operations and maintenance cost.

5. Implementation of Temoa

This section describes the implementation of the model formulation provided in Section 4. We have implemented Temoa within an algebraic modeling environment. Algebraic modeling languages (AML) like GAMS (Brooke and Rosenthal, 2003) or AMPL (Fourer et al., 1987) provide an intuitive method for model formulation, analogous to the notation associated with mathematical programming problems. A major advantage of AMLs is their ability to describe models distinctly from the data on which they operate (Kallrath, 2004). As a result, well-designed EEO model source code represents a generic energy optimization framework, which operates on specific datasets to produce results.

Our design goal was to assemble an open source software stack that enables uncertainty analysis in an HPC environment. We are utilizing the COmmon Optimization Python Repository (Coopr), a set of Python-based optimization utilities developed by Sandia National Laboratories (Hart and Watson, 2009). Temoa's core EEO model heavily utilizes two subcomponents of Coopr: an AMPL-like environment called Python Optimization Modeling Objects (Pyomo), and Python-based Stochastic Programming (PySP). Figure 8 includes key software elements and the links between them. Sections 5.1 and 5.2 describe the implementation of the Temoa model formulation using Pyomo and PySP, respectively.

¹Calculated as:
$$\frac{TDR_{t,v}}{1-(1+TDR_{t,v})^{-LLN_{t,v}}}$$

5.1. Programming Environment

The choice of application programmer interface (API) and environment is crucial to a project whose stated goal is transparency. We selected Pyomo for a number of reasons. Influenced by the design of AMPL, Pyomo is an open source Python library that provides capabilities commonly associated with algebraic modeling languages (AMLs) such as AMPL, AIMMS, and GAMS; however, Pyomo is also embedded within a full-featured high-level programming language with a rich set of supporting libraries (Hart, 2009). Pyomo leverages the Python component architecture to support extensibility in a modular manner. Modeling in a high level language allows modelers to utilize modern programming constructs, ensure cross-platform portability, and access the broad range of functionality found in standard software libraries. The benefits of using Python are twofold: (1) it serves as a robust, well-tested foundation for model development and (2) extensions generally require new classes or routines rather than changes to the language itself (Hart, 2009).

One drawback to Python and Pyomo over a standard AML is the verbosity of syntax. While a pure AML has syntax very close to actual mathematical notation, the generality of Python requires more overhead code (i.e., required code that does not directly relate to the math). We made the decision to sacrifice the conciseness of an AML for the power and flexibility of a general purpose programming language. Python is widely used in the scientific community (Pérez et al., 2011) and such broad familiarity with Python is an important consideration for a new modeling effort trying to appeal to modelers from a variety of disciplines. In addition, the algebraic formulation provided in Section 4 can be ported to a different programming environment in the future, if necessary.

The Temoa user documentation made available on the project website describes the model implementation in detail (Hunter et al., 2013). To encourage contributions back to the energy modeling community, all of Temoa's model-specific code is made available under the GNU Affero Public License (FSF, 2007).

5.2. Optimization Tools

A key strength of Coopr is that models developed in Pyomo can link to optimizers written in low-level languages (e.g., C and FORTRAN). This two-language approach leverages the flexibility of a high-level language for formulating optimization problems and the efficiency of low-level languages for numerical computations (Hart, 2009). Coopr links to several linear and mixed integer linear solvers, including CPLEX (Cplex, 2007), Gurobi (Bixby et al., 2010), CBC (Forrest and Lougee-Heimer, 2005), and GLPK (Makhorin, 2010).

Another strategic reason for using Coopr is the ability to link Temoa with solvers that can handle a variety of mixed integer and non-linear formulations. Future Temoa development may include a mixed integer or non-linear formulation to model endogenous technological change (Barreto, 2001; Manne and Barreto, 2004), non-linear macroeconomic production functions (e.g., Bauer et al., 2008), or use of the logit function as a market sharing algorithm (Short et al., 2007).

Coopr also contains Python-based Stochastic Programming (PySP), a modeling and solver library for generic stochastic programming (Watson et al., 2010). Modeling in PySP involves coupling a fully-specified event tree with a Pyomo-based deterministic, single-scenario model of the problem. The event tree specification includes the assignment of conditional probabilities and stochastic parameter values to each branch in the event tree.

PySP can also address instances where the extensive form is too difficult to solve, due either to the presence of integers (in any stage) or a sufficiently large event tree. In this case, PySP provides a generic and highly customizable scenario-based decomposition solver based on Rockafellar and Wets' Progressive Hedging algorithm, which has proved effective as a heuristic for difficult, multi-stage stochastic mixed-integer programs (Rockafellar and Wets, 1991). Because the progressive hedging algorithm decomposes a stochastic problem into the set of paths through the event tree, it is possible to implement the algorithm in a parallel computing environment.

6. Verification Exercise

With the algebraic model formulation and subsequent Pyomo implementation complete, we conducted a verification exercise to test model performance. Following the lead of Howells et al. (2011), we utilized

'Utopia', a simple test energy system bundled with ANSWER, a graphical user interface packaged with the MARKAL model generator (Noble, 2007). Utopia can deploy 17 technologies across three model time periods (1990, 2000, 2010) to meet 3 end-use demands: residential lighting (RL), residential space heating (RH), and automobile transportation (TX). Within each time period, a representative year is split into three seasons (winter, summer, intermediate) and two times of day (day, night). Among the three seasons, the average lighting and space heating demands are highest in the winter and higher in the day compared to night. Transportation demand remains constant throughout the year.

To meet these demands, the model can deploy and utilize a lighting technology (RL1), electric space heaters (RHE), oil-based space heaters (RHO), and electric, diesel, and gasoline cars (TXE, TXD, TXG). Coal combustion (E01), light water nuclear reactors (E21), hydroelectricity (E31), and oil combustion (E70) can generate electricity. A pumped hydroelectric facility (E51) is also available to store and dispatch electricity. The system receives fuel from the import of coal (IMPHCO1), uranium (IMPURN1), crude oil (IMPOIL1), gasoline (IMPGSL1), and diesel (IMPDSL1). Imported crude oil can be refined into gasoline and diesel via a refinery technology (SRE). Figure 8 provides the system network map.

Running the model produced the technology capacity results shown below in Figure 8. The objective function value, representing the present cost of energy supply, is \$36.5 billion in Temoa, and \$32.7 billion in MARKAL, which represents a 12% difference.²

Figure 8 indicates a discrepancy in the choice of space heating technology. The combined RHO and RHE capacity in Temoa is 62 and 93 PJ/year in 2000 and 2010. In MARKAL, the combined RHO and RHE capacity is 37.8 and 56.7 PJ/year in 2000 and 2010, respectively. Temoa is choosing to build more capacity than MARKAL because Equation (2), which defines the relationship between activity and capacity, requires it. To illustrate the difference, Table 2 presents the demand in each time slice as well as the length of each time slice, expressed as the fraction of a year (SEG). The bottom portion of the Table 2 represents the resultant demand device capacity required by MARKAL and Temoa.

The MARKAL demand device capacity required to meet a given end-use demand is equal to the sum of demand device activity. By contrast, Equation (2) in Temoa requires that the product of demand device capacity and the time slice length (SEG) be greater than or equal to its activity. As a result, the total demand device capacity required to meet a given end-use demand is higher in Temoa than MARKAL, as shown in Table 2. We assert that our approach is more accurate: To ensure that supply meets demand, the total rate of commodity production must equal the total rate of commodity demand. In turn, the rate of commodity demand – end-use demand per unit time – is given by the demand level in each time slice divided by the duration of each time slice. For example, RH demand rate in 2000 during winter-day is given by $20.7 \, \text{PJ} / 0.333 \, \text{year} = 62 \, \text{PJ/year}$. Since winter-day yields the highest demand rate across all six slices, it determines the total required capacity for heating technologies (RHO and RHE). MARKAL instead assumes that the required capacity for combined RHE and RHO is $37.8 \, \text{PJ/year}$, which does not account for the time slice length and implicitly assumes constant annual demand. For demands that remain constant throughout the year (e.g., TX), the MARKAL and Temoa capacity results match, as shown in Figure 8 for TXD and TXG. Dividing the TX demands by the appropriate SEG yields the same rate of demand in each time slice.

As a result, the MARKAL formulation results in an underinvestment in demand device capacity in cases where the demand rate (e.g., PJ/year) varies throughout the year. The underinvestment in MARKAL explains the discrepancy in the values of the Temoa and MARKAL objective functions presented above. To verify this conclusion, we formulated a second version of Temoa that calculates the demand device capacity by assuming constant annual demand. This is achieved by formulating a separate version of Equation (2) which does not include SEG on the left hand side of the equation, for all technologies except for electric generators. This version is able to identically replicate the MARKAL activity and capacity results, producing a Temoa objective function value of \$33.3 billion, which is 2% lower than the MARKAL result. This remaining discrepancy is due to the precise nature of the objective function calculation: Temoa first annualizes investment costs and then sums those annual payments over the future horizon, whereas

²Note that the MARKAL run was conducted with STARTYRS = 0, such that all costs are discounted to the beginning of the first period in order to be consistent with Temoa.

MARKAL assumes a lump sum investment cost, with a salvage value credited back to the objective function for capacity exceeding the specified future horizon.

The model source code and data used to generate results associated with the Utopia verification exercise are archived in our Git repository, accessible from the project website (Hunter et al., 2013). Note that the Temoa formulation resides in the energysystem branch, while the alternative formulation used to replicate the MARKAL result is archived separately in the exp_energysystem_match_MARKAL branch.

7. Stochastic Implementation of Utopia

Upon completion of the verification exercise, we tested the functionality of PySP by implementing a stochastic version of the Utopia system. The simplicity of the Utopia system and our familiarity with it through the model verification process made it a logical choice as a proof-of-concept test of Temoa's stochastic optimization capability. Suppose that Utopia is an island state and is gravely concerned with fuel supply over the next three decades. Due to geopolitical concerns and a lack of domestic resources, the prices of imported crude oil, diesel, gasoline, and coal are expected to increase dramatically from 2000 through 2019, corresponding to the 2000 and 2010 model time periods. Energy planners in Utopia would like to prepare a strategy that is contingent on the possible future price rates. The crude oil, diesel, and gasoline are imported from the same location, and therefore the low, medium, and high growth rates for all three fuels are assumed to be the same and follow identical growth patterns. The assumed import price growth rates are provided in Table 3.

The resultant event tree considers each combination of growth rates for coal and liquid fuels, resulting in 9 branches per node implemented across two time stages with uncertainty for a total of 81 scenarios. For simplicity, each branch is assigned an equal probability of (1/9), or roughly 11%. The deterministic version of the model (i.e., source code and base case data file) along with the event tree information was passed to PySP, which constructed the extensive form of the stochastic problem and invoked CPLEX to find the optimal solution. Figure 8 is a scatterplot of the total discounted system cost – the objective function value – as a function of the average coal price from 2000 to 2019. The marker shading is proportional to the imported price of oil, diesel, and gasoline, where lighter shades indicate higher prices. Figure 8 indicates how total energy expenditures in Utopia vary under the 81 different fuel price scenarios.

The variation in results can be observed by choosing two extreme scenarios within the event tree and examining the technology results. Figure 8 provides the activity associated with both fuel imports and demand devices in the Utopia system when coal prices are highest and liquid fuel prices are lowest (left bars), and vice versa (right bars). Since there is no modeled uncertainty in 1990, the results in all scenarios are the same and represent a near-term hedging strategy that accounts for the modeled future outcomes weighted by their probabilities. The 1990 results indicate that Utopia should maintain a balance between imports of coal, diesel, and gasoline, with coal used for electricity generation (E01), diesel for space heating (RHO), and gasoline for vehicles (TXG). If coal prices remain high relative to imported oil, diesel, and gasoline prices, as in the left bars of Figure 8, Utopia should consider fuel switching in its electric sector to nuclear by 2010. If coal prices are low relative to imported oil, diesel, and gasoline prices, as in the right bars of Figure 8, Utopia should consider a sharp increase in coal imports in order to ramp up electricity production. The additional electricity can be used to supplant oil heaters (RHO) with electric heaters (RHE) and to displace a portion of the gasoline vehicles (TXG) with electric vehicles (TXE). The hedging strategy suggests a moderated approach to fuel imports in 1990, followed by recourse options over the following two decades depending on how uncertainty in fuel prices imports are revealed.

While this stochastic exercise with Utopia is simply a proof-of-concept for the Temoa framework, the ability to conduct stochastic optimization with much larger datasets in an HPC environment can lend valuable insight into the planning process by allowing the construction of complex event trees that account for multiple parameter uncertainties. Note that Temoa's stochastic version of Utopia draws on the source code and data available in the energysystem branch, supplemented with files made available in the stochastic subdirectory.

8. Discussion

Two primary needs drive the design of Temoa: greater transparency in EEO modeling and rigorous assessment of future uncertainty. Towards transparency, Temoa draws on a large, existing ecosystem of open source software components, and is itself an open source project. Temoa utilizes an open source AML-like environment, Pyomo, to implement the algebraic formulation, links to open source solvers (e.g., GLPK), and is archived in an electronically and publically accessible RCS. The use of Pyomo allows us to conduct sensitivity and uncertainty analysis in a HPC environment, thereby enabling parallel processing of model runs required for parametric sensitivity analysis, Monte Carlo simulation, and stochastic optimization (via PySP). In particular, the ability to conduct stochastic optimization with more complex event trees can better inform decision makers who must take action on energy and environmental issues before future uncertainty is resolved.

The verification exercise using the 'Utopia' system presented in Section 6 demonstrates that the Temoa model formulation and implementation are correct. The observed discrepancy between MARKAL and Temoa regarding the calculation of demand device capacity demonstrates the utility of careful verification exercises. The comparison unearthed a simplification in the MARKAL formulation that can lead to underinvestment in technology capacity. Despite its simplicity, the stochastic optimization of Utopia represents a proof-of-concept application of Temoa. Further, public access to our RCS allows interested parties to use the archived model source code and data, and more importantly, to reproduce our published results. For example, those interested in reproducing our Utopia results can access a snapshot of the source code and data within the web accessible repository, linked from the Temoa Project website (Hunter et al., 2013).

Over time, we fully expect that changes will be made to the model formulation. The formulation presented here represents a single snapshot archived in our publicly accessible RCS, but as we update the formulation, changes will be integrated into the documentation available on the project website. In addition, we plan to use the RCS to archive distinct versions of the model formulation with different capabilities, tuned to the needs of particular analyses. Keeping the model codebase as small as possible for a particular application will maintain model transparency by allowing modelers and users to interrogate model source code and data with greater ease. While the implementation in Pyomo is more verbose than other algebraic modeling languages such as GAMS or AMPL, we hope that Temoa will benefit the energy modeling community.

Ongoing work by the authors is focused on methodological improvements in the application of stochastic optimization, while external collaborators at Carnegie Mellon and Princeton Universities are conducting studies related to U.S. natural gas supply, energy development on an American Indian reservation, and energy futures in India.

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References

Babonneau, F., Haurie, A., Loulou, R., Vielle, M., 2012. Combining Stochastic Optimization and Monte Carlo Simulation to Deal with Uncertainties in Climate Policy Assessment. Environmental Modeling and Assessment, 1–26.

Balaji, P., Buntinas, D., Butler, R., Chan, A., Goodell, D., Gropp, W., Krishna, J., Latham, R., Lusk, E., Mercier, G., Ross, R., Thakur, R., 2011. MPICH2 User's Guide. Tech. Rep. Version 1.4.1, Argonne National Laboratory, Office of Science, U.S. Department of Energy.

Balay, S., Brown, J., Buschelman, K., Eijkhout, V., Gropp, W. D., Kaushik, D., Knepley, M. G., McInnes, L. C., Smith, B. F., Zhang, H., 2011. PETSc Users Manual. Tech. Rep. ANL-95/11 - Revision 3.2, Argonne National Laboratory.

Barnes, N., 2010. Publish Your Computer Code: It Is Good Enough. Nature 467 (7317), 753-753.

Barreto, L., 2001. Technological Learning in Energy Optimisation Models and Deployment of Emerging Technologies. Ph.D. thesis, National University.

Bauer, N., Edenhofer, O., Kypreos, S., 2008. Linking Energy System and Macroeconomic Growth Models. Computational Management Science 5 (1), 95–117.

Bhatt, V., Friley, P., Lee, J., 2010. Integrated Energy and Environmental Systems Analysis Methodology for Achieving Low Carbon Cities. Journal of Renewable and Sustainable Energy 2 (03).

Bixby, R., Gu, Z., Rothberg, E., 2010. Gurobi Optimization.

Bosetti, V., Tavoni, M., 2009. Uncertain R&D, Backstop Technology and GHGs Stabilization. Energy Economics 31, S18–S26. Brooke, A., Rosenthal, R. E., 2003. GAMS. GAMS Development.

Clarke, L., Edmonds, J., Jacoby, H., Pitcher, H., Reilly, J., Richels, R., Jul 2007. Scenarios of Greenhouse Gas Emissions and Atmospheric Concentrations. U.S. Department of Energy Publications.

URL http://digitalcommons.unl.edu/usdoepub/6

Cplex, I., 2007, 11.0 User's Manual, ILOG SA:.

Craig, P. P., Gadgil, A., Koomey, J. G., 2002. What Can History Teach Us? A Retrospective Examination of Long-Term Energy Forecasts for the United States. Annual Review of Energy and the Environment 27 (1), 83–118.

DeCarolis, J. F., 2011. Using Modeling to Generate Alternatives (MGA) to Expand Our Thinking on Energy Futures. Energy Economics 33 (2), 145–152.

DeCarolis, J. F., Hunter, K., Sreepathi, S., Jul 2012. The Case for Repeatable Analysis with Energy Economy Optimization Models. Energy Economics 34 (6), 1845–1853.

EIA, 2012. Annual Energy Outlook 2012. Tech. Rep. DOE/EIA-0383(2012), Office of Integrated Analysis and Forecasting, U.S. Department of Energy, U.S. Government Printing Office, Washington, D.C., U.S. Energy Information Administration (EIA).

Ellson, J., Gansner, E., Koutsofios, L., North, S., Woodhull, G., 2002. Graphviz – Open Source Graph Drawing Tools. In: Graph Drawing. pp. 594–597.

Fishbone, L. G., Abilock, H., Jan 1981. MARKAL, a Linear Programming Model for Energy Systems Analysis: Technical Description of the BNL Version. International Journal of Energy Research 5 (4), 353–375.

Forrest, J., Lougee-Heimer, R., 2005. Cbc user guide. INFORMS Tutorials in Operations Research, 257-277.

Fourer, R., Gay, D. M., Kernighan, B. W., 1987. AMPL: A Mathematical Programming Language. AT&T Bell Laboratories. FSF, Nov 2007. GNU Affero General Public License. Version 3. Free Software Foundation (FSF), Boston, MA, USA. (Accessed Apr. 2013).

URL https://www.gnu.org/licenses/agpl-3.0.html

Gritsevskyi, A., Nakićenovi, N., Nov 2000. Modeling Uncertainty of Induced Technological Change. Energy Policy 28 (13), 907–921.

Hanson, B., Sugden, A., Alberts, B., 2011. Making Data Maximally Available. Science 331 (6018), 649-649.

Hart, W. E., 2009. Python Optimization Modeling Objects (Pyomo). Operations Research and Cyber-Infrastructure, 3-19.

Hart, W. E., Watson, J.-P., 2009. Coopr: a COmmon Optimization Python Repository Sandia National Laboratories, Albuquerque, NM, USA.

URL http://software.sandia.gov/coopr/

Holthausen, D. M., Dec 1979. Hedging and the Competitive Firm Under Price Uncertainty. The American Economic Review 69 (5), 989–995.

Howells, M., Rogner, H., Strachan, N., Heaps, C., Huntington, H., Kypreos, S., Hughes, A., Silveira, S., DeCarolis, J., Bazillian, M., Roehrl, A., Oct 2011. OSeMOSYS: The Open Source Energy Modeling System: An Introduction to Its Ethos, Structure and Development. Energy Policy 39 (10), 5850–5870.

Hunter, K., DeCarolis, J., Sreepathi, S., 2013. Tools for Energy Modeling Optimization and Analysis. (website), (Accessed Apr, 2013).

URL http://temoaproject.org/

IEA, 2010. Energy Technology Perspectives 2010: Scenarios and Strategies to 2050. Organisation for Economic Cooperation and Development, Paris, France, OECD. Publishing and International Energy Agency.

Ince, D. C., Hatton, L., Graham-Cumming, J., 2012. The Case for Open Computer Programs. Nature 482 (7386), 485–488.

Kainuma, M., Matsuoka, Y., Morita, T., 1998. Analysis of Post-Kyoto Scenarios: The AIM Model. In: Economic Modeling of Climate Change: OECD Workshop Report.

Kallrath, J., 2004. Modeling Languages in Mathematical Optimization. Vol. 88. Springer.

Kann, A., Weyant, J. P., 2000. Approaches for Performing Uncertainty Analysis in Large-Scale Energy/Economic Policy Models. Environmental Modeling & Assessment 5 (1), 29–46.

Kanudia, A., Loulou, R., 1998. Robust Responses to Climate Change via Stochastic MARKAL: The Case of Québec. European Journal of Operational Research 106 (1), 15–30.

Labriet, M., Loulou, R., Kanudia, A., d'études et de recherche en analyse des décisions (Montréal, Québec), G., 2008. Is a 2 Degrees Celsius Warming Achievable Under High Uncertainty?: Analysis with the TIMES Integrated Assessment Model. Groupe d'études et de recherche en analyse des décisions.

Lamport, L., 1986. LaTeX: A Document Preparation System, 2nd Edition. Addison-Wesley Longman Publishing Co., Inc., Boston, MA, USA.

Loulou, R., Goldstein, G., Noble, K., et al., 2004. Documentation for the MARKAL Family of Models. IEA Energy Technology Systems Analysis Programme.

Loulou, R., Kanudia, A., 1999. Minimax Regret Strategies for Greenhouse Gas Abatement: Methodology and Application. Operations Research Letters 25 (5), 219–230.

Loulou, R., Lehtila, A., 2007. Stochastic Programming and Tradeoff Analysis in TIMES. IEA ETSAP TIMES version 2.

Loulou, R., Remme, U., Kanudia, A., Lehtila, A., Goldstein, G., 2005. Documentation for the TIMES Model PART I. Energy Technology Systems Analysis Programme. Disponível.

Lutz, M., Sep 2009. Learning Python, 4th Edition. O'Reilly.

Makhorin, A., 2010. GNU Linear Programming Kit: Reference Manual for GLPK Version 4.45 38, Department for Applied Informatics, Moscow Aviation Institute. Moscow, Russia.

Manne, A. S., Barreto, L., Jul 2004. Learn-by-Doing and Carbon Dioxide Abatement. Energy Economics 26 (4), 621-633.

Messner, S., Strubegger, M., 1995. User's Guide for MESSAGE III. Rep. WP-95-69, International Institute for Applied Systems Analysis, Laxenburg, Austria.

- Morgan, M. G., Henrion, M., 1990. Uncertainty: A Guide to Dealing with Uncertainty in Quantitative Risk and Policy Analysis. New York, New York, USA.
- Morgan, M. G., Keith, D. W., 2008. Improving the Way We Think about Projecting Future Energy Use and Emissions of Carbon Dioxide. Climatic Change 90 (3), 189–215.
- Morris, S. C., Goldstein, G. A., Sanghi, A., Hill, D., 1996. Energy Demand and Supply in Metropolitan New York with Global Climate Change. Annals of the New York Academy of Sciences 790 (1), 139–150.
- Morrison, M., Morgan, M. S., 1999. Models as Mediating Instruments. IDEAS IN CONTEXT 52, 10–37.
- MPICH2, Mar 2013. MPICH2. (webpage), (Accessed Apr, 2013).

URL http://www.mpich.org/

- Nakićenović, N., Alcamo, J., Davis, G., de Vries, B., Fenhann, J., Gaffin, S., Gregory, K., Grubler, A., Jung, T. Y., Kram, T., et al., 2000. Special Report on Emissions Scenarios: A Special Report of Working Group III of the Intergovernmental Panel on Climate Change. Cambridge University Press, New York, NY (US), Pacific Northwest National Laboratory, Richland, WA (US), Environmental Molecular Sciences Laboratory (US).
- Noble, K., 2007. ANSWER v6 MARKAL User Manual: ANSWER MARKAL, an Energy Policy Optimization Tool. Noble-Soft Systems Pty Ltd, Australia.
- Nordhaus, W. D., 1993. Rolling the DICE': An Optimal Transition Path for Controlling Greenhouse Gases. Resource and Energy Economics 15 (1), 27–50.
- Pérez, F., Granger, B., Hunter, J., 2011. Python: An Ecosystem for Scientific Computing. Computing in Science & Engineering 13 (2), 13–21.
- PETSc, Jun 2012. Portable, Extensible Toolkit for Scientific Computation. (website), (Accessed Apr, 2013). URL http://www.mcs.anl.gov/petsc/
- Ravetz, J., 2003. Models as Metaphors. Public Participation in Sustainability Science: A Handbook, 62Cambridge University Press.
- Rockafellar, R. T., Wets, R. J. B., 1991. Scenarios and Policy Aggregation in Optimization Under Uncertainty. Mathematics of Operations Research, 119–147.
- Short, W., Ferguson, T., Leifman, M., 2007. Modeling of Uncertainties in Major Drivers in US Electricity Markets. NREL. UCAR, Mar 2013. Community Earth System Model (CESM). (website), University Corporation for Atmospheric Research
 - URL http://www.cesm.ucar.edu/

(UCAR).

- Watson, J.-P., Woodruff, D. L., Jul 2010. Progressive Hedging Innovations for a Class of Stochastic Mixed-Integer Resource Allocation Problems. Computational Management Science 8 (4), 355–370.
- Watson, J. P., Woodruff, D. L., Hart, W. E., 2010. PySP: Modeling and Solving Stochastic Programs in Python. Tech. rep., Technical report, Sandia National Laboratories, Albuquerque, NM, USA.
- Weyant, J. P., 1993. Costs of Reducing Global Carbon Emissions. The Journal of Economic Perspectives 7 (4), 27–46.

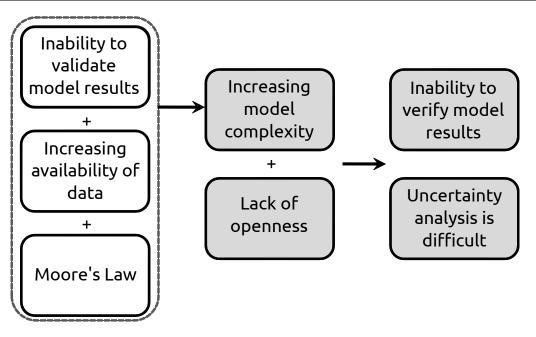


Figure 1: Causal model that highlights the limitations associated with the prevailing approach to EEO model development and application. The Temoa project aims to address the issues highlighted in gray.

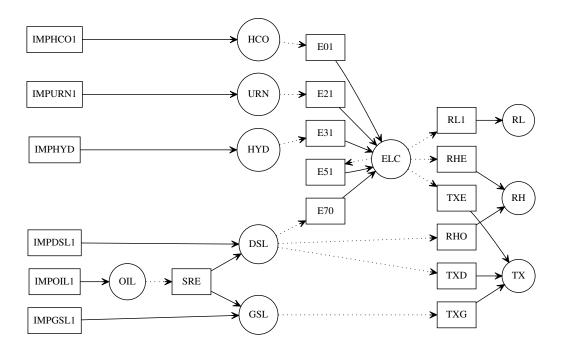


Figure 2: Energy system map associated with the 'Utopia' energy system used for model verification. Energy technologies are represented by boxes and energy commodities by circles. The dotted lines represent the commodity flow into each technology (**FI**); the solid lines represent commodity flow out (**FO**).

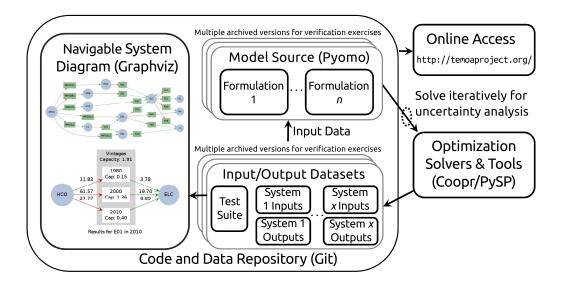


Figure 3: A schematic of the open source software elements utilized by Temoa, and the linkages between them. Git is used as the revision control system, providing public access to model source code and input data archives. Model formulations 1...n and datasets 1...x emphasize that multiple copies of source code and data can be stored in the repository, each pertaining to a different analysis.

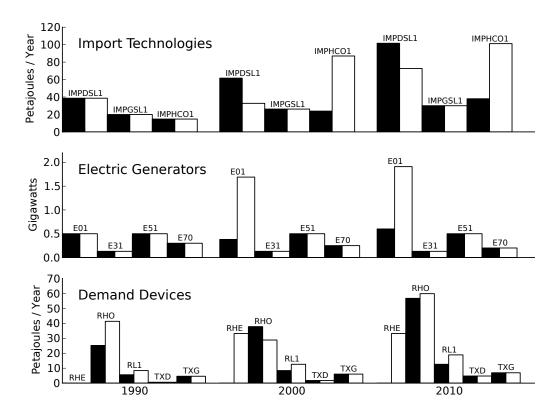


Figure 4: Technology capacity in each model time period for both MARKAL and Temoa using the 'Utopia' test system. Black and white represent MARKAL and Temoa results, respectively. Names above each set of black-white bars indicate the technology name. Note that Temoa requires higher capacities for demand devices serving end-use demands that vary by season and time-of-day. The difference in the required capacity for demand devices drives the discrepancies in results between MARKAL and Temoa.

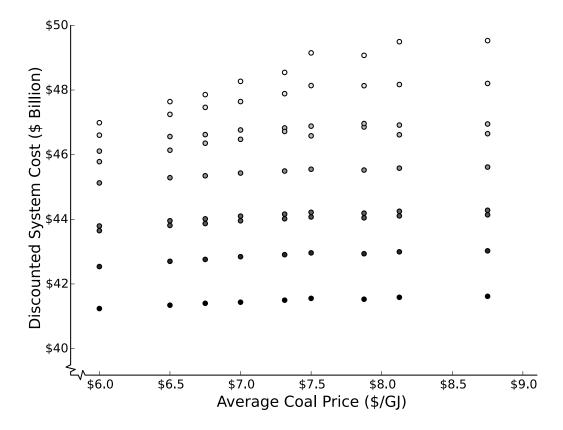


Figure 5: Total discounted system cost as a function of the average imported coal (HCO) price across the 2000 and 2010 time periods. The shade of each point is proportional to the average imported price of crude oil, diesel, and gasoline over the same periods, and all three fuels follow identical growth patterns. Lighter shades indicate higher import prices. Note the suppressed zeros; the variation in total system cost is roughly 20%.

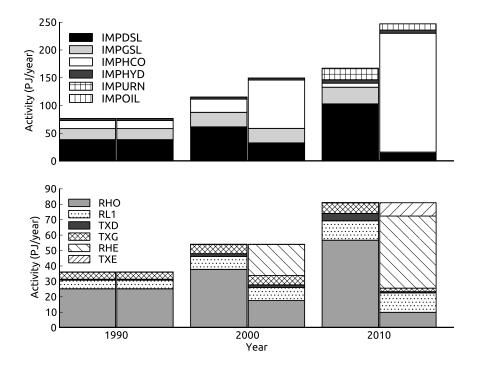


Figure 6: Results associated with fuel imports (top) and the energy produced by demand devices (bottom) for two scenarios drawn from the stochastic Utopia run. For each time period, the left bars correspond to the scenario with the highest coal prices and lowest oil, diesel, and gasoline prices; the right bars correspond to the scenario with the lowest coal prices and highest oil, diesel, and gasoline prices.

Table 1a: List and Description of Temoa's Set Nomenclature

	Class Control of Tomore Section of Tomore Sectio
Set	Short Description
$c \in C$	C is the set of all user-defined commodities
$C^d \subset C$	C^d is a subset of (C) that includes only the demand commodities, i.e., the commodities representing end-use demands
$C^e \subset C$	C^e is a subset of (C) that includes only the emissions commodities, i.e., the commodities representing pollutant emissions
$d \in D$	D is the set of all diurnal time segments (d)
i = c	i is an alias for c , representing the commodity input to a technology
o = c	o is an alias for c , representing the commodity output from a technology
P^e	set of periods that define technology vintages existing prior to the future period set (P^f)
$p \in P^f$	model periods of interest; each element marks the <i>beginning</i> of a period; the last element specifies the last year of the horizon, not the beginning of another period
$v \in V$	V is the set of all technology vintages (v) ; a vintage is defined by the model time period (p) in which a technology (t) is installed; $V = P^e \cup P^f$
$s \in S$	S is the set of all user-defined seasons (s)
$t \in T$	T is the set of all user-defined technologies (t)
$T^b \subset T$	T^b is a subset of (T) that includes only baseload electric technologies, i.e., thermal power plants that do not adjust output diurnally
$T^d \subset T$	T^d is a subset of (T) that includes only demand technologies, i.e., the technologies directly serving an end-use demand.
$T^r \subset T$	T^r is a subset of (T) that includes only resource technologies, i.e., the technologies that represent the extraction or import of natural resources
$T^s \subset T$	T^s is a subset of (T) that includes only the storage technologies, which balance storage and dispatch across the set of daily time segments (D)
Θ	Sparse superset representing allowable combinations of set elements. The subscript to Θ uniquely identifies the superset associated with each equation.

Table 1b: List and Description of Temoa's Parameter Nomenclature

	able 1b. List and Description of Temoa's Farameter Nomenciature			
Parameter	Short Description			
$C2A_{t,v}$	parameter that converts capacity units to activity units			
$CF_{s,d,t,v}$	capacity factor of a process that can vary by season and time of day			
$DEM_{p,c}$	end-use demands specified by period and commodity			
$DSD_{s,d,c}$	Percentage distribution of demand c , per time slice			
$EAC_{e,i,t,v,o}$	emissions rate of process based on input / output commodity pair			
$ECAP_{t,v}$	amount of pre-existing process capacity prior to P^f			
$EFF_{i,t,v,o}$	conversion efficiency; based on input / output commodity pair			
$ELM_{p,e}$	emissions limit specified per period			
$FC_{p,t,v}$	fixed operations and maintenance cost			
GDR	global discount rate used to calculate present value of future period costs			
$IC_{t,v}$	process investment cost			
$LA_{t,v}$	*loan amortization factor to convert future lump sum investment costs to annualized			
,	amounts; based on TDR			
LEN_p	*calculated number of years in period $p \in P^f$			
$LLN_{t,v}$	*process-specific loan term			
$MAX_{p,t}$	upper bound on capacity installation by model time period			
$MIN_{p,t}$	lower bound on capacity installation by model time period			
$MLL_{t,v}$	*lesser of the following: number of years until the end of process loan life or the final year in the P^f horizon			
$MTL_{p,t,v}$	*lesser of the following: number of years until the end of process lifetime or the final year in the P^f horizon			
$RSC_{p,c}$	upper bound on resource commodity production			
$SEG_{s,d}$	fraction of year represented by each combination of season (s) and time-of-day (d)			
$SPL_{i,t,o}$	fraction of total input commodity (i) converted to the output commodity (o) through technology (t)			
$TDR_{t,v}$	technology-specific discount rate used to calculate LA. Defaults to GDR if not specified			
$TLF_{p,t,v}$	*fraction of period p that a process is active			
$VC_{p,t,v}$	variable cost			

^(*) Temoa automatically determines the indices and values of these parameters.

Table 1c: List and Description of Temoa's Variable Nomenclature

	<u> </u>
Variable	Short Description
$\mathbf{FI}_{p,s,d,i,t,v,o}$	commodity flow into a process to produce a given output, per time slice
$\mathbf{FO}_{p,s,d,i,t,v,o} \ \mathbf{ACT}_{p,s,d,t,v}$	commodity flow out of a process based on a given input, per time slice
$\mathbf{ACT}_{p,s,d,t,v}$	total commodity production of a process, per time slice
$\mathbf{CAP}_{t,v}$	process capacity required to support all associated activity
$\mathbf{CAPAVL}_{p,t}$	total capacity available of technology t in period p ; not necessarily a simple vintage
$CAIAVL_{p,t}$	summation because of the TLF parameter

Table 2: Utopia Demand Data and MARKAL and Temoa Results

Table 2. Ctopia Belliana Bata and William Enda Temoa Testatis							
Time Slice	CEC	RL		RH		TX	
Time since	$\mathbf{SEG}_{s,d}$	2000	2010	2000	2010	2000	2010
Intermediate-Day	0.167	1.26	1.89	4.54	6.80	1.30	1.95
Intermediate-Night	0.083	0.42	0.63	2.27	3.40	0.65	0.97
Summer-Day	0.167	1.26	1.89	0	0	1.30	1.95
Summer-Night	0.083	0.42	0.63	0	0	0.65	0.97
Winter-Day	0.333	4.20	6.30	20.7	31.0	2.60	3.90
Winter-Night	0.167	0.84	1.26	10.3	15.5	1.30	1.95
MARKAL Capacity		8.40	12.6	37.8	56.7	7.80	11.69
Temoa Capacity		12.6	18.9	62.0	93.0	7.80	11.69

Table 3: Decadal Growth Rates Used in Stochastic Utopia

Import Prices	Low	Medium	High
Coal	200%	225%	250%
Oil, Diesel, Gasoline	125%	150%	175%