System Integration with Multiscale Networks (SIMoN): A Geo-Temporal Model Transformation Framework for a Sustainable Future

***Abstract*—With the rise of globalization, climate change, population growth, and resource depletion, new modeling techniques are needed to assess the sustainability of our future resources. These methods must adapt to many highly coupled domains, accommodate new models and data as they emerge, facilitate validation through model comparison, and handle the patchwork of data and models available with different units, definitions, and geo-temporal scales. Here we propose a new modeling framework, which addresses these challenges through System Integration with Multiscale Networks (SIMoN). The SIMoN framework connects predictive resource models from different domains, and uses a ZeroMQ-based messaging system to pass resource utilization and availability data between models. Each model takes discrete time steps and runs in its own Docker container to increase flexibility and scalability.**

SIMoNs novelty stems from its treatment of geographic regions. Geographies are defined by a partially ordered set of geographic partitions, with a corresponding directed acyclic graph to organize numerous compatible shapefiles. SIMoN enables users to define consistent aggregation and disaggregation maps for transformation between disparate notions of geography (e.g., counties, watersheds, and power regions). These transformations are performed on-the-fly and only as needed by wrappers around each model. This unique approach to geographic transformation will provide flexible tools to tie models together across domains.

***Index Terms*—Model Transformation, Geography, Sustainability, Resource Modeling, Model Communication.**

I. Introduction

HERE we introduce a new framework- System Integration with Multiscale Networks (SIMoN)- for joint model runs. SIMoN addresses the challenge of data transformation between models with disparate geographic (or temporal) definitions. The SIMoN framework assists modelers in predicting the availability of critical resources such as power, water, and food in the future. The framework will also incorporate population and climate change models, as these are strong drivers for resource demand and availability. These domains each come with their own hierarchies of geography which include political, topographical, regulatory, and coordinate grid induced boundaries. We outline a plan to combine these many definitions into a general notion of geography.

SIMoN provides tools for the modeler to integrate new models and geographic definitions easily. The modeler selects transformation functions, called aggregators and disaggregators, to move the data between compatible geographic definitions. These aggregators and disaggregators must conform to a set of axioms provided, which are chosen to create a provable notion of data consistency across geographies. The framework is designed to be extensible and flexible, including tools to enable the introduction of new domains and corresponding geographies. Examples in this paper will focus on geography, but these definitions extend naturally to disparate definitions of time.

II. Previous Work

Integrated approaches to modeling the food-energy-water (FEW) nexus have been increasing for the past decade or two. For instance, Lubega and Farid created a physics-based model for the water-energy nexus using the Systems Modeling Language (SysML) [1]. Additionally, Tidwel et al [2] created a system dynamics model for integrated management and decision support of electrical and water systems in the US. Some efforts even brought together siloed decision support modeling systems for a more integrated approach. For example, Yates and Miller [3] linked the Water Evaluation and Planning (WEAP) modeling system [4] with the Long Range Energy Alternatives Planning (LEAP) system for integrated energy and water planning.Most recently, Endo et al [5] provided an overview of research in the area of food, energy, and water, including tools developed for modeling and analysis.

Current approaches to modeling FEW and related systems are generally tailored to the subset of systems that they address and are not designed for adaptation to new or different models within these sectors. As such, they also do not address between-model differences in geography or time scales that may occur when marrying two or more models that were not initially designed to work together or that were developed in isolation. Further, due to the complicated nature of the interactions between systems, as well as the enormous extent of each individual system, many researchers focus on two of these systems at a time [6]. Additionally, current approaches do not aim at developing a flexible framework that would allow further systems to be included in analysis, but rather focus on development of individual models and their interactions.

There are more general modeling and simulation tools used in this space, though none filling the gaps that SIMoN aims to fill. For instance, consider Dymola [7], a component modeling tool that models physical parts and thus operates at a lower level than SIMoN. The General Algebraic Modeling System (GAMS) [8] is a powerful optimization tool that does not aid modellers in handling different time and geography scales. The Climate, Land, Energy, and Water (CLEW) modeling framework [9] is more similar to SIMoN in that it is concerned with resource modeling in order to identify relationships between sectors and how to minimize trade-offs. It may be used at different geographic scales, though models in each sector must agree on a single geography scale. The Multi-scale integrated analysis of societal and ecosystem metabolism

(MuSIASEM) [10] allows for modeling at multiple scales with a focus on the performance of socioeconomic activities and ecological constraints in order to understand and analyze resource use by society and the impacts to the environment. The Global Change Assessment Model (GCAM), developed as a collaboration between the University of Maryland and the Pacific Northwest National Laboratory (PNNL), is another integrated assessment tool for exploring the impacts of global change [11], [12]. Unlike SIMoN, the individual GCAM models, as well as the time and geography scales are fixed within the larger GCAM model. Furthermore, simultaneous solvers couple the GCAM domains tightly. The SIMoN approach allows the user to more flexibly combine models without simultaneously solving over the same geographic regions.

III. Model Assumptions and Initial Models

SIMoN models are assumed to work together to predict the supply, demand, or distribution of resources in the future using discrete time steps.

The goal of SIMoN is to provide tools for combining existing models. Thus, initial SIMoN experiments have used publicly available data sets and relatively simple Python models for proof-of-concept. The intention is to open source the framework and populate a domain model library with many alternative models for each domain. The framework captures the most important interactions between these models in the interface described in Section IV: Software Framework. Models currently implemented for demonstration include:

- A county-level population model extrapolating U.S. Census data [13] using the Holt's linear trend method [14]. This model predicts county-level populations from the previous years' data.
- A simple model of power demand was created based on total state-level power sales [15]. This model estimates the per capita demand for each state based on the year 2016. These state-level coefficients are currently assumed to be constant and are used to calculate future demand as a function of state population.
- A model of power generation assumes that generation always meets demand for each power region, specifically the North American Electric Reliability Corporation (NERC) regions, then constructs a power production profile based on the generation-weighted profile of power plants within a NERC region. This profile is generated using U.S. EIA plant-level emissions and water consumption data [16]. This model calculates the quantity of emissions (CO2 and NOx) generated per megawatt-hour (MWh) and water consumption from power plant cooling per MWh for each NERC region based on data from 2016.

For incorporation in the next few months we will include:

- A simple Python climate change model, SimMod [17], which predicts the global mean temperature by taking in global emissions data.
- Models based on either a higher fidelity climate models such as Hector [18], or based on the outputs of Global Climate Model (GCM) runs such as GFDL-CM3 [19]. Results of these runs are based on representative concentration pathways (RCPs) which represent scenarios of time dependent greenhouse gas concentration projections and can have outputs of near-surface air temperature, precipitation, and evaporation.
- A new Python model for accounting for available water in the contiguous United States. The model follows the general guidelines that are used to determine water resource budgets for each area as described by the Michigan Water Resources Department assuming a steady state water budget [20]. Water availability is derived from input (rainfall) and consumption (evaporation, evapotranspiration, and human use) for each Hydrologic Unit Code 8 (HUC8) watershed [21] and transfers any unused water for a given year into the next downstream watershed.

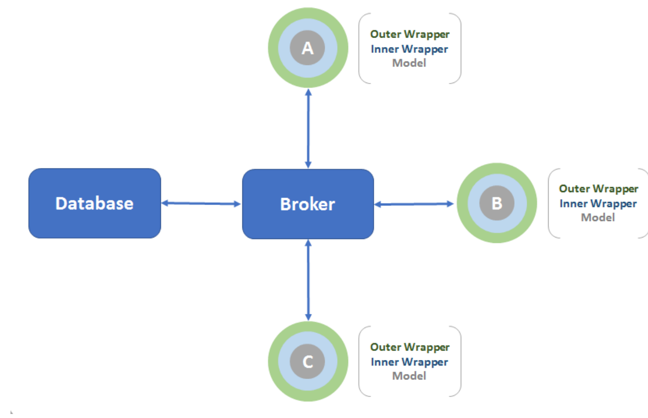

Fig. 1. SIMoN Framework Architecture

It is up to the modeler running the SIMoN framework to decide which models to use and how these models should interact within the framework. The examples of data exchange given here can be enriched or reduced.

IV. Software Framework

The SIMoN framework is designed to be modular, extensible, and flexible to a variety of black box models. A diagram of the system architecture is included in Figure 1. Each model runs in a separate Docker container enabling different models in the framework to have conflicting dependencies. A universal outer wrapper operates in each model container to standardize the model interface with the system. This outer wrapper will also perform the data transformations described in SectionVIII. A central broker, also in its own container, orchestrates model runs and initiates the first time step. After each time step, the models publish their data in JSON format using ZeroMQ. The broker archives these data messages in a backend database for post processing. New models can be introduced into the framework by building a docker image that can execute the model. The user must also construct an inner wrapper which translates the model inputs and outputs into their respective JSON schemas, which include an attribute for geographic granularity. These granularities are constructed in Section VI

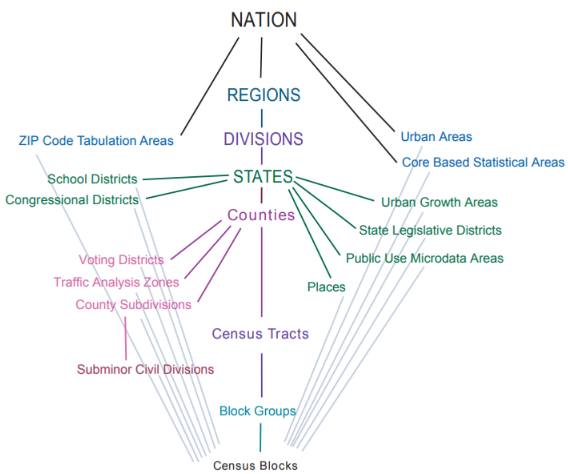

Fig. 2. Census Bureau Hierarchy from www.census.gov

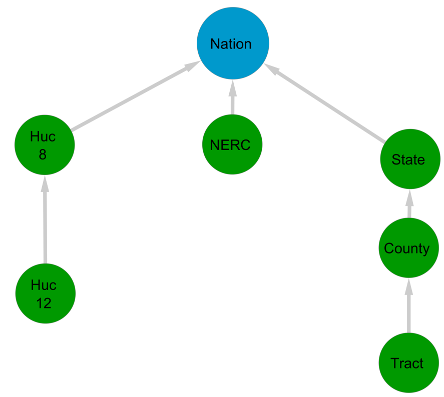

Fig. 3. A small Hasse Diagram D_P with political, water, and power regions

V. Geographic Definitions

The SIMoN framework is designed to capture the interactions between domains such as power, water, population, climate, and food. Each of the domains modeled in SIMoN has its own definitions of geography. In fact, domains tend to have entire hierarchies of geography associated to them, as this is a natural way to organize data collection and curation. For example, the U.S. Census Bureau organizes its data collection into a hierarchy displayed in Figure 2.

While we wish to be flexible to many definitions of geography, we must establish some rules for allowable geographies to enable data transformations. It is required that all models in a given simulation using the SIMoN framework operate on the same overall geographic region called the **scope** (e.g. the United States). Any data outputs shared by a model for the consumption of other models in SIMoN must include data for the entire scope. Each model, however, may have different definitions of how that scope is subdivided. In particular, any data set can be shared on any finite partitions of the scope. Elements of the partition are non-overlapping subsets of the scope, where the union of these elements is the entire scope. Examples of partitions include counties, watersheds, NERC or other power regions, lat/lon grid overlays, map pixels, etc. For the purpose of initial demonstration, the examples that follow will use the contiguous United States as their geographic scope. Many of the region types captured in the Census Bureau Hierarchy are examples of partitions of this scope. However, Urban Areas are NOT a partition of the United States, since not every point in the United States is contained in an Urban Area. A model concerned with Urban Areas would have to be extended (even if that extension is trivial) in order to operate with other models over the contiguous United States within SIMoN.

Given multiple partitions of geography, some will be naturally compatible in that they represent refinements of others. Given two partitions $X = \{x_i\}_{i=1}^n$ and $Y = \{y_j\}_{j=1}^m$ of the same scope S, we say that Y is a refinement of X if $\forall y_j \in Y$, $\exists\, x_i \in X$ such that $y_j \subseteq x_i$. For example, counties are a refinement of states, because both partition the contiguous United States and each county is contained in a single state. Note: in our geographic implementation, the partition of counties and the partition of states both contain a special element representing the District of Columbia to satisfy the partition properties, and parishes are considered as counties for Louisiana.

VI. Abstract Geography Construction

We construct a sequence of directed graphs of geography to create a reference tool for models to communicate through the framework. These graphs and functions defined on their edges organize the data transformations between model geographies and are used to define a global notion of data transformation consistency.

Any set of partitions of the scope S forms a partially ordered set, or poset, where the binary relation $\leq$ is given by $Y \leq X$ if and only if Y is a refinement of X. It is straightforward to check that this operation is reflexive, antisymmetric, and transitive. This partially ordered set can be represented uniquely by its Hasse Diagram: a directed acyclic graph (DAG) where the vertices represent partitions and an edge $Y \rightarrow X$ is inserted if and only if Y is a refinement of X. We select the convention of always drawing the finest partitions at the bottom. The trivial partition of the scope is a supremum always drawn at the top. In general, we will define P to be the partially ordered set of the scope and its partitions of interest, that is- those partitions of geography which represent possible data granularities in SIMoN. An example P is given in Figure 3, represented by the corresponding Hasse Diagram D_P. We can see in Figure 3 how the right arm of this definition parallels the hierarchy of the Census Bureau, although our edges are much more meaningful.

Given a P representing the scope S and its geographies of interest from the data/mode perspective, we construct an augmented DAG, Q, which includes a new element, the meet $X \wedge Y$, for every pair of incomparable elements $X, Y \in P$.

The purpose of constructing the meet is to define a new geography which serves as a bridge between its parent elements. Each $X \wedge Y$ inserted is a new, unique partition of geography of the maximal regions which still allow $X \wedge Y$ to be a refinement

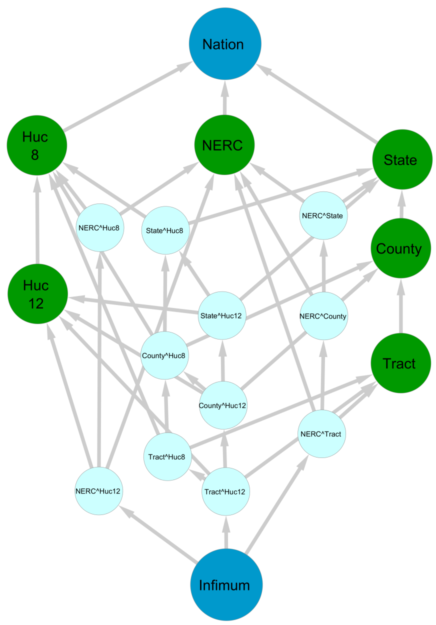

Fig. 4. The Hasse Diagram of D_P has been extended to the DAG G_Q with vertex meets and edges of interest. Pairwise meets are indicated in light blue.

of both X and Y. Visually, if the boundary lines of X and Y are overlaid on the same map, all bounded regions are elements of the partition $X \wedge Y$. Because X and Y are partitions, for each region $z \in X \wedge Y$, $\exists$ unique $x_i \in X, y_j \in Y$ such that $z = x_i \cap y_j$. We call x_i and y_j the parents of z, just as we call X and Y the parents of $X \wedge Y$.

Note that if $Y \leq X$ in the poset P, $X \wedge Y = Y$ is also in P. A new element is not inserted in Q. Also the operation of meet is symmetric so $\forall X, Y \in P, X \wedge Y = Y \wedge X$. So if $|P| = n$, then $|Q| \leq n - 1 + \binom{n-1}{2}$.

We associate to Q an abstract DAG, G_Q, as follows.

1) If (X, Y) is an edge in G_P, then (X, Y) is in G_Q.
2) For every $X \wedge Y \in Q$, there are two edges, $(X, X \wedge Y)$ and $(Y, X \wedge Y)$.
3) If there is an edge (X, Y) in G_P, and $Z \in P$, there is an edge from $(X \wedge Z, Y \wedge Z)$ in G_Q.

Note that under this construction, G_Q has too many edges to be the Hasse diagram of Q, but it contains it.

Finally, we add an infimum element INF to Q that is the meet of all childless nodes, with corresponding edges in G_Q. The graph G_Q is our final definition of the relationships between notions of geography, and is called the **Abstract Geography Graph**.

The advantage of constructing these pairwise and universal meets will be that they provide bridges for transforming data between the geographic definitions of different models. In particular, to transform data from geographic granularity A to granularity B, it is necessary to follow the undirected path $(A, A \wedge B)(A \wedge B, B)$, using operations defined in Section VIII. The universal meet, while not directly involved in any data transforms, will be useful in checking the consistency of geography and function definitions.

VII. Constructing Geospatial Data and Instance Graphs

The directed graphs representing abstract definitions of geographies and their relationships in the previous section have real world instantiations of interest to modelers. We will assume that $\forall X \in P$ representing a model-driven definition of geography, there is a shapefile SF_X that fully defines the regions of X within the scope S. For example, if X is states in the contiguous United States, then SF_X will be a shapefile with 49 distinct regions. We represent each of these regions as a node in the **Instance Geography Graph** I_P. The instance graph has the same general structure as the abstract geography graph, except that every individual vertex in the abstract graph has been replaced by many vertices. For example, rather than a single vertex representing 'states' in our political boundary graph, there would be 49 vertices of type 'state' representing the forty-eight contiguous states and the District of Columbia. Each of these states has a directed edge into the single element of the scope/supremum. Similarly, the node 'county' is replaced with 3108 vertices of type 'county', each with an edge to its unique parent of type 'state'.

Constructing the instance graph I_P corresponding to P is computationally quick, since it is assumed that a shapefile is provided for every vertex $X \in P$ in each of the shapefiles that correspond to the pairwise meets $X \wedge Y$ where $X, Y \in P$ can be accomplished more efficiently by iterating from top to bottom, and using the graph structure to reduce the intersections computed. Instance graphs grow large quickly, so computing them up front can provide a significant savings to the modeler. For example, the instance graph for a partially ordered set containing only the elements Nation, State, County, and NERC Region is shown in Figure 5.

VIII. Aggregation and Disaggregation Definitions

Let Y be an element of the abstract geography graph G_Q. Let $\vec{v}_Y$ be a vector of length $|Y|$ representing a data value defined for all vertices of type Y in the instance graph I_Q. For example, $\vec{v}_Y$ may represent the population of each county at time t where Y is the vertex 'county', or the rainfall in each watershed region where Y represents the vertex 'HUC8'.

We define an **aggregation operator** A to be a collection of functions, one for each directed edge (V, W) in G_Q that take data defined on the instances of W to data defined on the instances of V. Write the function associated to the (V, W) as $A_{\{W:V\}}$, where $A_{\{W:V\}} : \mathbb{R}^{|W|} \to \mathbb{R}^{|V|}$. These functions aggregate data from a refinement, such as counties, to a higher level, such as states. We will not assume that these functions can be represented by matrix multiplication, although this is the case for many important examples. The most common aggregation operator will sum the data over the children of a node in the instance graph I_Q. For example, the population of a state for the power demand model will be calculated by summing the populations of its child counties which are output by the population model. However, not all aggregations are sums. For example, to aggregate the maximum power load over a set of child nodes in the instance graph, the aggregation operator MAX would be used.

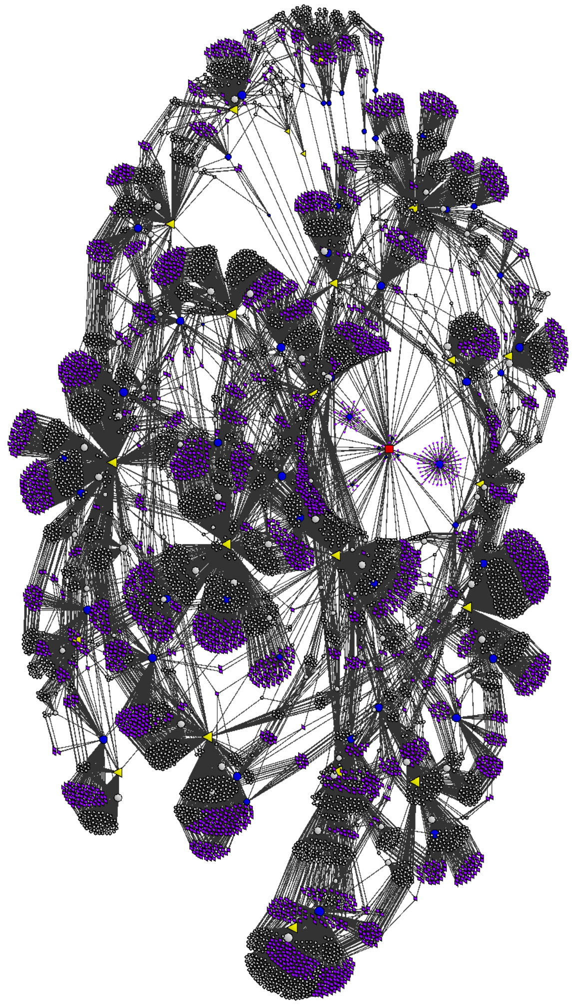

Fig. 5. This instance graph I_Q includes the scope of the contiguous United States (red square), NERCS (yellow triangles), states (blue circles), and counties (purple circles), as well as the intersections of NERC and counties (grey vertices). The overlapping nature of states and NERCS can be seen.

Aggregation Notation: Let $Y \leq X$ in Q. If $\vec{v_Y} \in \mathbb{R}^{|Y|}$ is the data associated to Y, then $\vec{v}_X = A_{\{Y:X\}}(\vec{v}_Y)$ is the data associated to X by aggregation operator A.

Similarly, a **disaggregation operator** D is a collection of functions, $D_{\{V:W\}}$, on edge (V, W) that takes data on V to data on W: $D_{\{V:W\}} : \mathbb{R}^{|V|} \to \mathbb{R}^{|W|}$. These functions disaggregate from a node to a refinement. The following are common examples of disaggregation functions on the instance graph I_Q:

- The constant map which populates each instance child node with a copy of the data from its parent
- Subdividing a data quantity among children according to a known ratio, such as the area of each child region

Disaggregation Notation: Let $Z \leq Y$ in Q. If $\vec{v_Y} \in \mathbb{R}^{|Y|}$ is the data associated to Y, then $\vec{v}_Z = D_{\{Y:Z\}}(\vec{v}_Y)$ is the data associated to Z by disaggregation operator D.

We say that the operators (A, D) form a valid **aggregation-disaggregation pair** on G_Q if and only if they satisfy the following axioms:

1) **Consistency**: For $Y \leq X$ in Q, and any $x_i = y_j$, the aggregators and disaggregators are the identity on the j^{th} and i^{th} components respectively:
$\forall \vec{v}_Y \in \mathbb{R}^{|Y|}, \quad \vec{v}_X[i] := A_{\{Y:X\}}(\vec{v}_Y)[j] = \vec{v}_Y[j]$
$\forall \vec{v}_X \in \mathbb{R}^{|X|}, \quad \vec{v}_Y[j] := D_{\{X:Y\}}(\vec{v}_X)[i] = \vec{v}_X[i]$
2) **Left Inverse**: $\forall Z \leq Y, A_{\{Z:Y\}} \circ D_{\{Y:Z\}} = \mathrm{id}_{\mathbb{R}^{|Y|}}$.
3) **Transitivity**: $\forall X \leq Y \leq Z \in Q, D_{\{X:Z\}} = D_{\{Y:Z\}} \circ D_{\{X:Y\}}$

The example operators listed below form valid pairs (A, D). The proof is left to the reader:

- (the constant map, MAX)
- (subdividing a data quantity among children according to the area of each, SUM)

These definitions provide a coherent mechanism for transferring a data vector between any two partitions. Suppose we are given partitions $X, Y \in Q$ and a data value $\vec{v}_X \in \mathbb{R}^{|X|}$ that we want the system to publish for partition Y. In general, we extend the data $\vec{v}_X$ to all of Q using a valid aggregator and disaggregator pair, (A, D). By construction, G_Q also contains $X \wedge Y$. We obtain $\vec{v}_{X\wedge Y} = D_{\{X:X\wedge Y\}}(\vec{v}_X)$, then apply $A_{X\wedge Y:Y}$ get the data vector $\vec{v}_Y \in Y$. That is, $\vec{v}_Y = A_{\{X\wedge Y:Y\}} \circ D_{\{X:X\wedge Y\}}(\vec{v}_X)$. The axioms ensure consistency on any region z that is part of X and Y. In particular, if $X = Y$, then we obtain the original data vector.

A different aggregation-disaggregation pair may be defined by the modeler for each data variable exchanged over the SIMoN framework. These mappings will be used by the outer wrappers that surround each model to transform data between geographies as needed. As more modelers implement valid transformation pairs, the library of recommended pairs will grow. We further plan to implement tools to check that potential new operator pairs satisfy the axioms listed here. Algorithmic approaches to the efficient construction of the data structures and consistency checks proposed are currently under development.

IX. Conclusion

This paper demonstrates the need to extend hierarchical approaches to modeling geography to more flexible posets of partitions, which can be used to build consistent data transformations between models. The current software implementation of the SIMoN framework includes functions which use geospatial data to construct abstract graphs, instance graphs, and geospatial data files for meets. The directed acyclic graphs and geospatial data created provide a shared language for geography across all models in the framework. The outer wrapper that surrounds each model tags data recorded with its level of geographic granularity. As data is received by other models, their outer wrappers will perform data transformations as needed using a consistent Aggregation-Disaggregation pair selected for each variable. This new approach to data transform can be applied to many domains where geographies are inconsistent. The SIMoN framework will also be extended to temporal transformations, constructing graphs that capture the interactions of time windows such as days, weeks, months, years, seasons, and billing cycles.

While the resource models incorporated into SIMoN for test are relatively simplistic, they demonstrate our ability to perform geographic transformation. We plan to expand the SIMoN Domain Model Library to include more complex fidelic models, additional domains such as food, and international models with larger overlapping scopes. The modular SIMoN framework will be used for a range of experiments comparing models and their interactions. Model perturbations which represent new policies or technologies can be incorporated into the framework easily, ultimately allowing decision makers to better understand the long-term impacts of their interventions on resource availability.

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