SYSTEMS ENGINEERING RESEARCH CENTER

UNIVERSITY OF MARYLAND 1856

SE4AI: Design of Digital Twins Architectures that Support AI and Machine Learning Formalisms working Side-by-Side as a Team

Sponsor: OUSD(R&E) | CCDC

By

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AI4SE/SE4AI Workshop

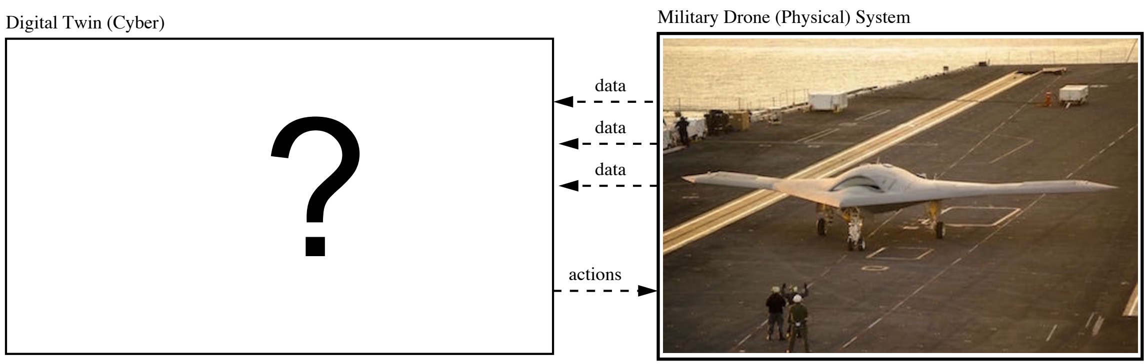
www.sercuarc.org

Cleared for Public Release

Digital Twins

Definition (2000 – today)

- Virtual representation of a physical object or system that operates across the system lifecycle (not just front end).



Required Functionality

- Mirror implementation of physical world through real-time-monitoring and synchronization of data with events.
- Provide algorithms and software for observation, reasoning and physical systems control.

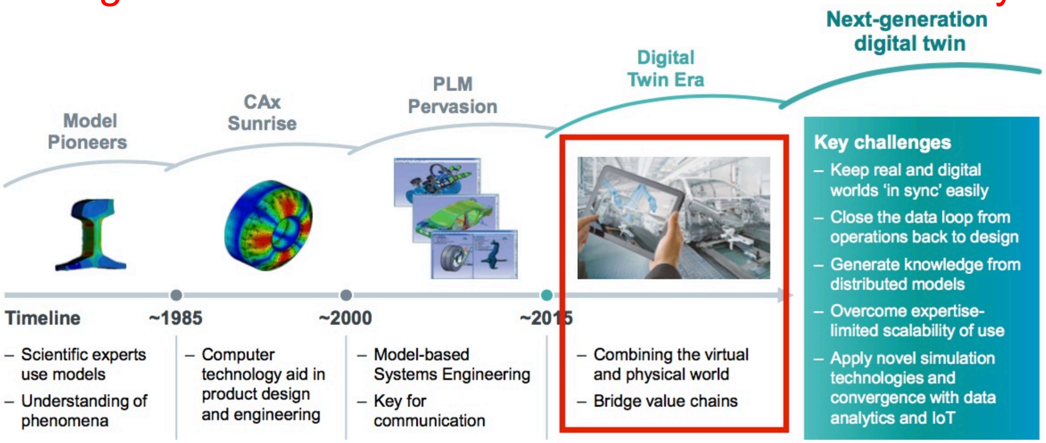
Many Application Domains

- NASA, manufacturing processes, building operations, personalized medicine, smart cities, among others.

Project Importance and Timeliness (Why?)

Business Drivers (Why this project is timely?)

Siemens, IBM, now see Digital Twin Era as the successor to MBSE with SysML



Digital Twin Era (Business Spin)

- New methods and tools for model-centric engineering.
- New operating system environments for observation, reasoning and physical systems control.
- Superior levels of system performance, agility, economy, etc.

Technical Implementation (2020, Google, Apple, Amazon, Siemens, IBM …)

- AI and ML will be deeply embedded in new software and algorithms.

Proposed Approach (Why?)

Definition of AI and ML

- AI: Knowledge representation and reasoning with ontologies and rules. Construction of semantic graphs, executable event-based processing, multi-domain reasoning.
- ML: Modern neural networks (closely related to signal processing of data streams). Data Mining. Input-to-output prediction, Learn structure and sequence. Identify objects, events, anomalies. Remember stuff.

AI/ML Strengths and Weaknesses

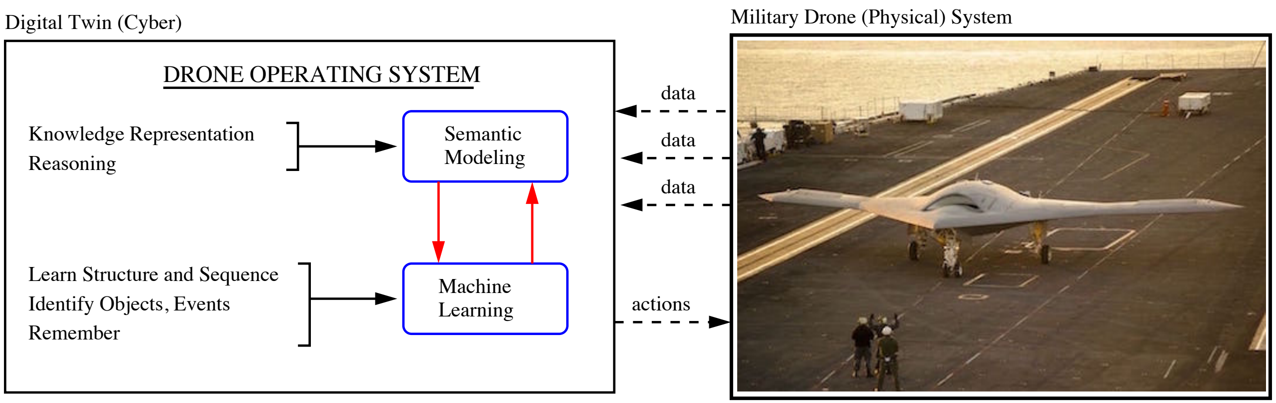
State-of-the-art AI and ML technologies are fragmented in their capability:

- AI provides a broad view of concepts needed for reasoning. Decision making processes are transparent; semantic graphs are flexible.
- Semantic reasoning is decision making in-the-moment (no memory).
- Data mining algorithms can organize information from large data sources.
- ML procedures developed to solve very specific tasks.
- ML decision making procedures lack transparency.
- ML procedures can identify anomalies (events) in streams of data.

Post Incubator Project (What's New?)

Digital Twins (What's New?)

- Explore design of digital twin architectures that support AI and ML formalisms working side-by-side as a team.



Key Research Challenge

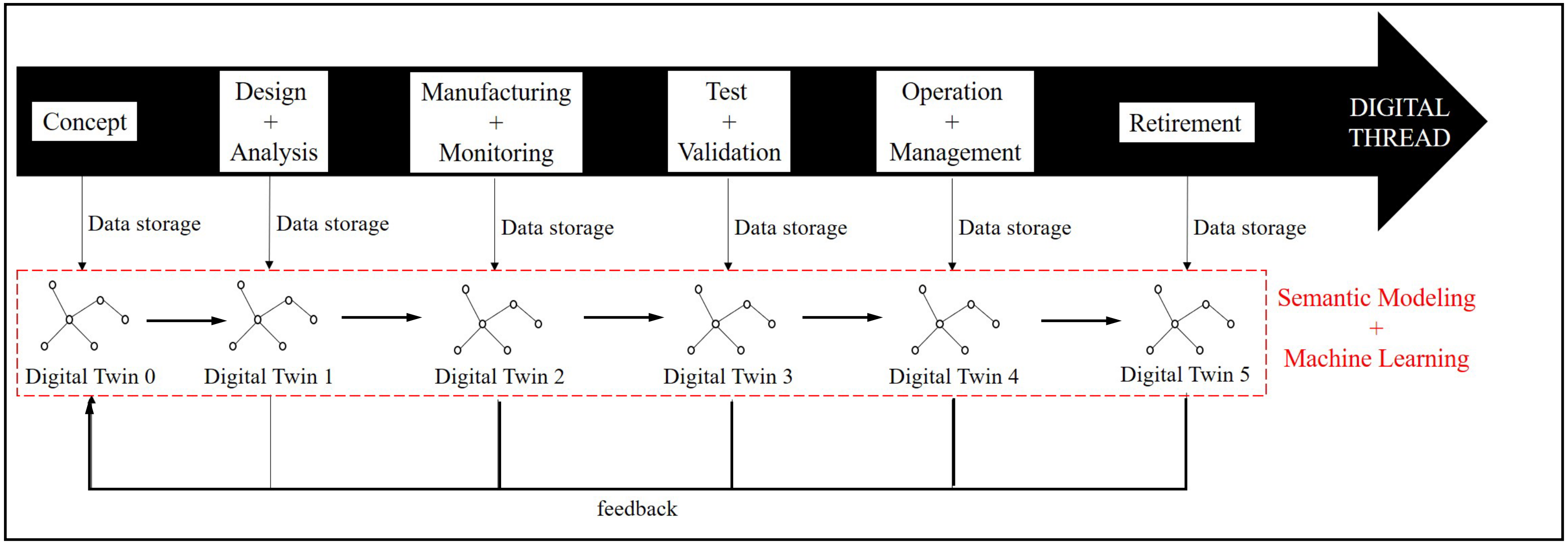
- How to design digital twin elements and their interactions to support: (1) methods and tools for model-centric engineering, and (2) digital twin operating system environments for observation, reasoning, control.

Project Success (What does it look like?)

- Knowledge to guide architectural development of future digital twins enabled by AI / ML technology.

Post Incubator Project (What?)

Cradle-to-Grave Lifecycle Support (Digital Threads)



Observation: A lot of model-centric engineering boils down to representation of systems as graphs and sequences of graph transformations punctuated by decision making and work / actions.

Reasonable Starting Point: Understand the range of possibilities for which machine learning of graphs and their attributes support and enhance activities in model-centric engineering and systems operation.

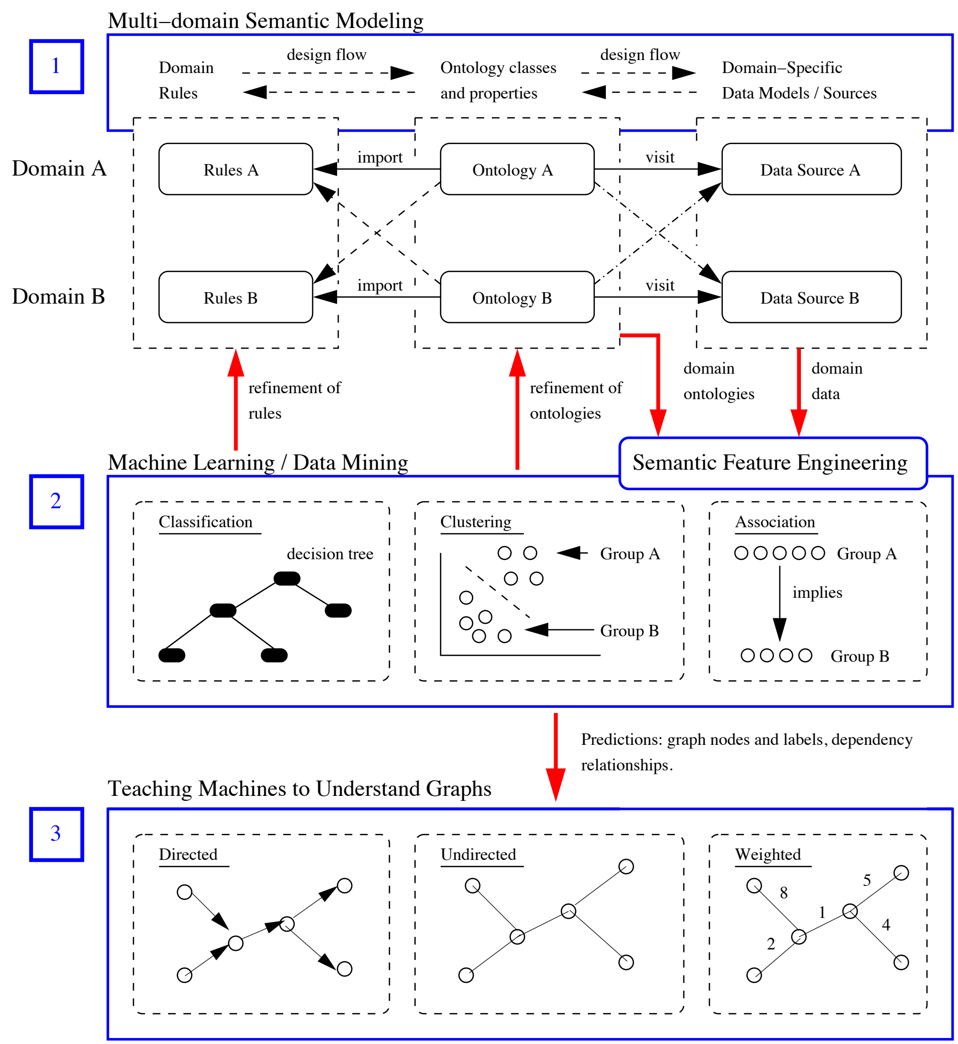
Example: Cross Domain Relationships Needed for System Trades, Analysis and Design

- Mission objective: continuous surveillance
- Capability Refueling UAV
- Systems: UAV and Refueler
- **<u>Valve</u>** – Cross-domain Object
- Mechanical Domain
  - Valve connects to Pipe
- Electrical Domain
  - Switch opens/closes Value
  - Maybe software
- Operator Domain
  - Pilot remotely sends message to control value
- Communication Domain
  - Message sent through network
- Fire control Domain
  - Independent detection to shut off valve
- Safety Domain

Post Incubator Project (What and How?)

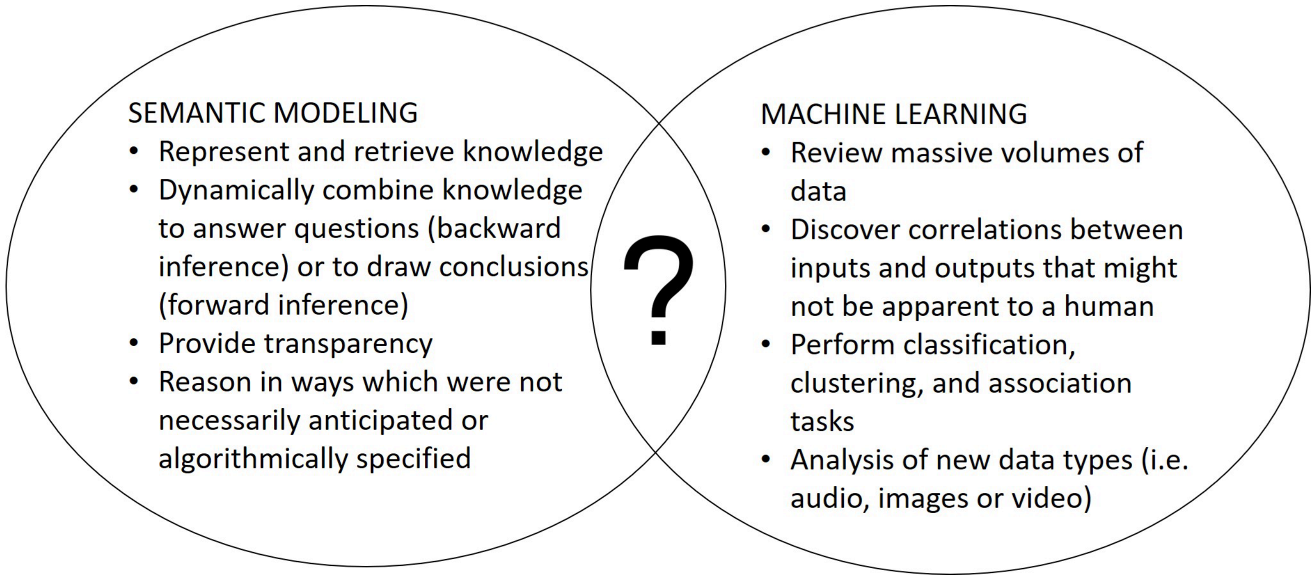
- Business Drivers
- Post Incubator Project
- Real-World Considerations
- **Step 1:** Multi-Domain Semantic Modeling
- **Step 2:** Semantic Modeling + Data Mining
- **Step 3:** Teaching Machines to Understand Graphs
- Opportunities and Extensions
- Plan of Work

So what will the machine learning do?



Initial Research Questions (low hanging fruit)

- What types of graphs (e.g., undirected, directed, weighted, multi-graph) are easy for the ML to learn?
- What can the ML do that is outside the capability of semantic modeling? And vice-versa?



- How can the ML improve the semantic modeling? And vice-versa?
- How to design the interactions connecting layers 1, 2 and 3
- How well do these techniques work with graph topology and attributes that are dynamic?

Semantic Modeling + Machine Learning

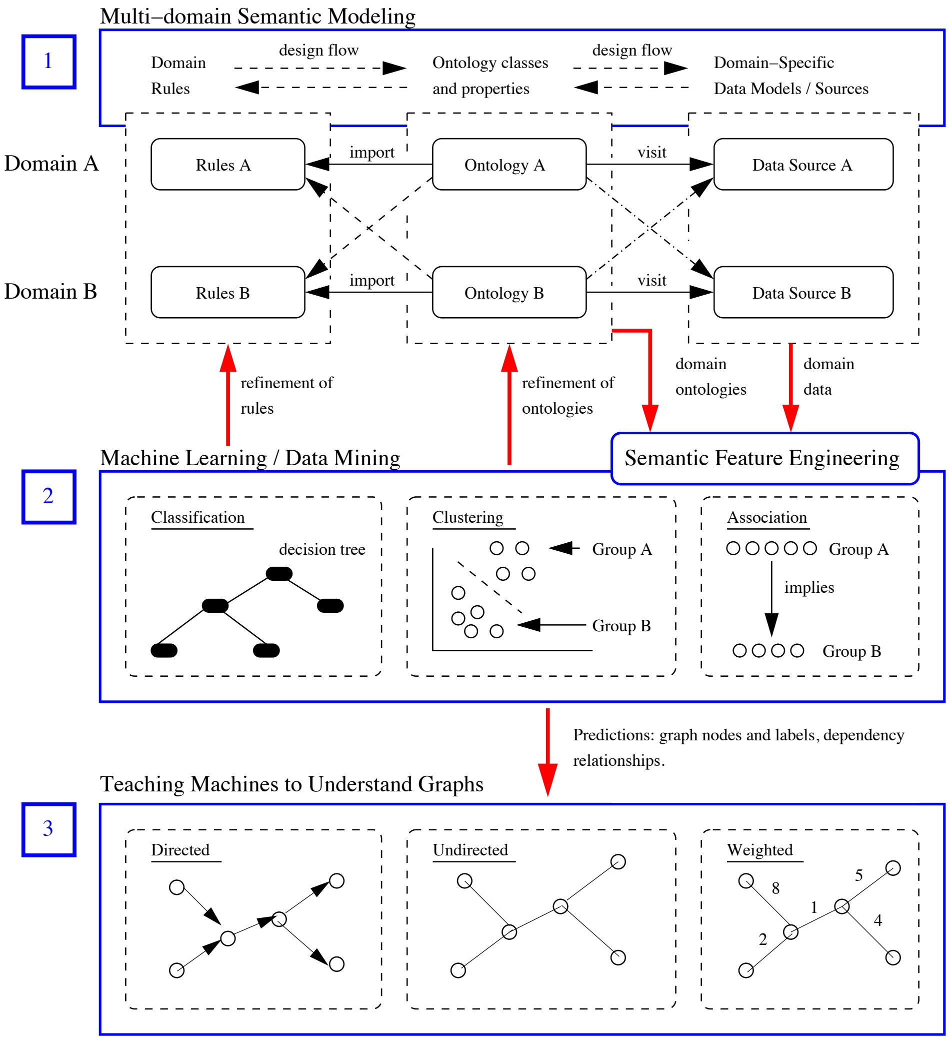
Semantic Modeling + Machines Trained to Understand Graphs

Is this even possible?

What will the machine learning do?

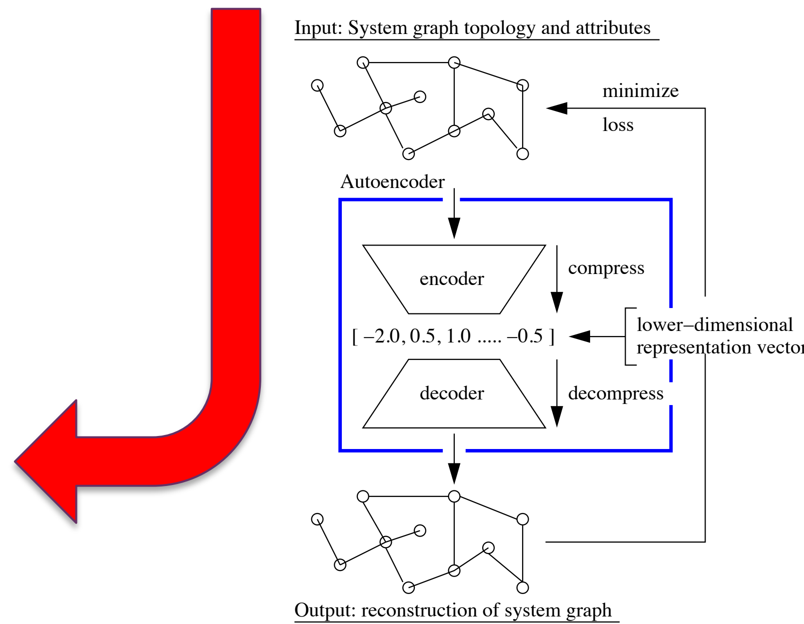
Post Incubator Project

Focus on Machine Learning of Graphs and Model-Centric Engineering.



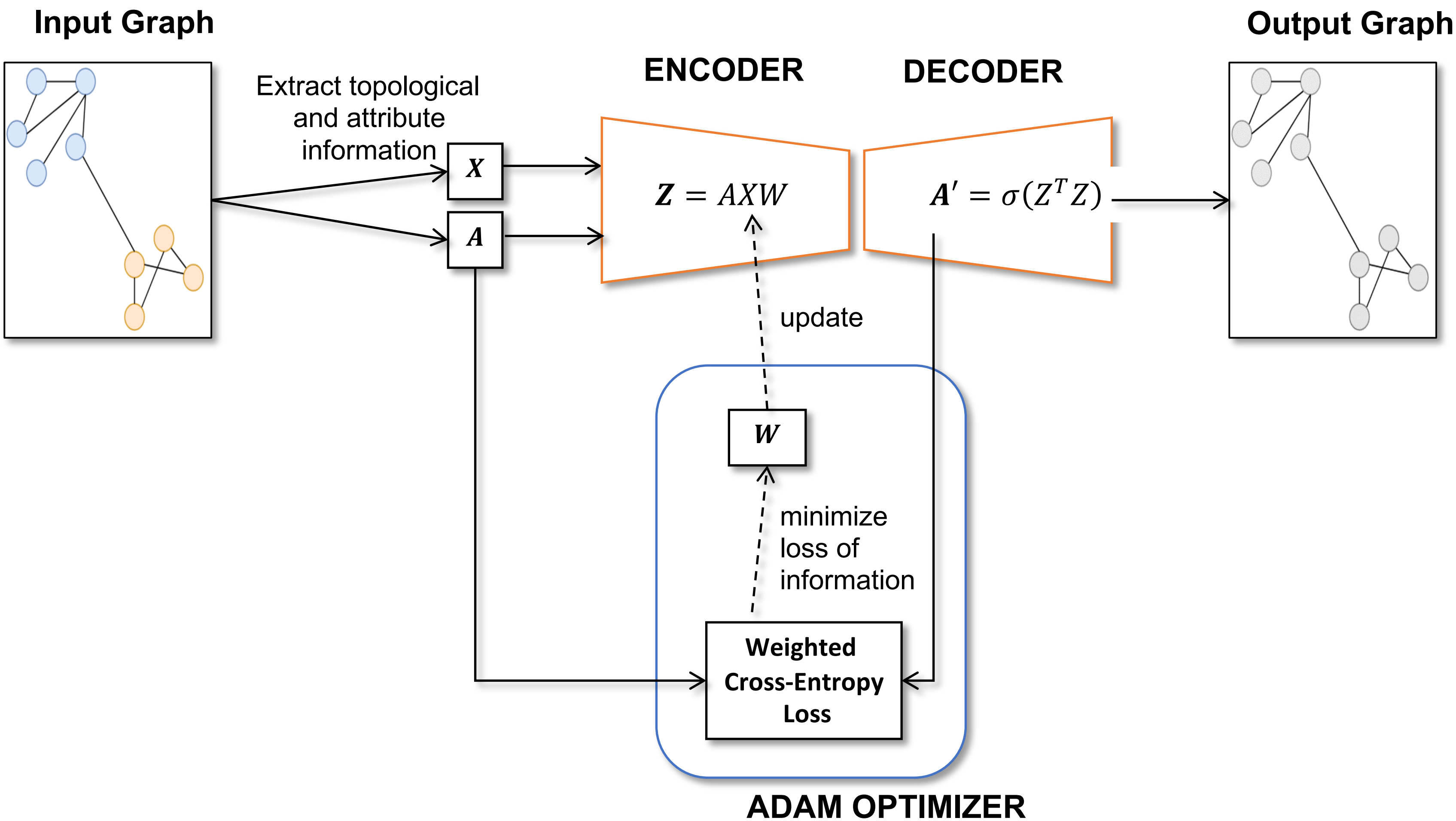
Observation: A lot of model-centric engineering boils down to representation of systems as graphs and sequences of graph transformations punctuated by decision making and work / actions.

Hence: Explore opportunities for training machines to understand graphs.



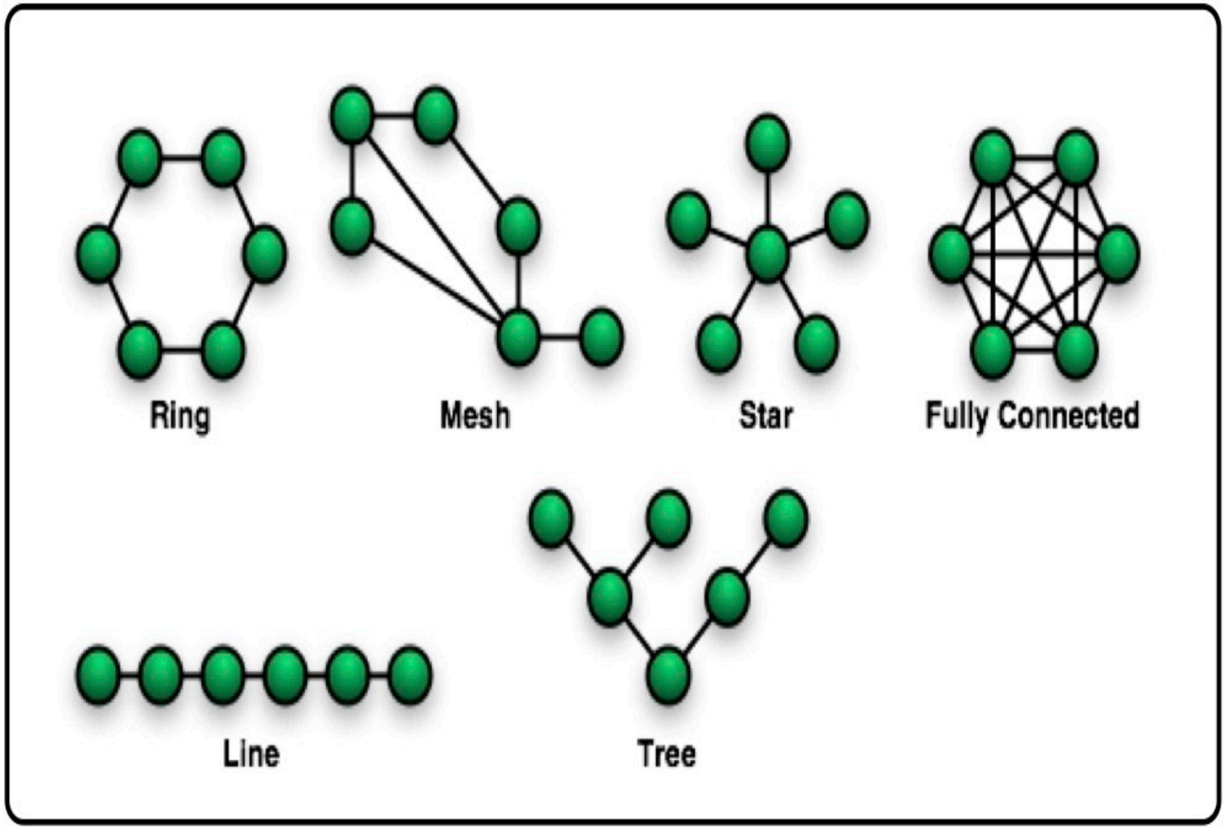
Teaching Machines to Learn the Topology of Graphs

Graph Auto-Encoding Process

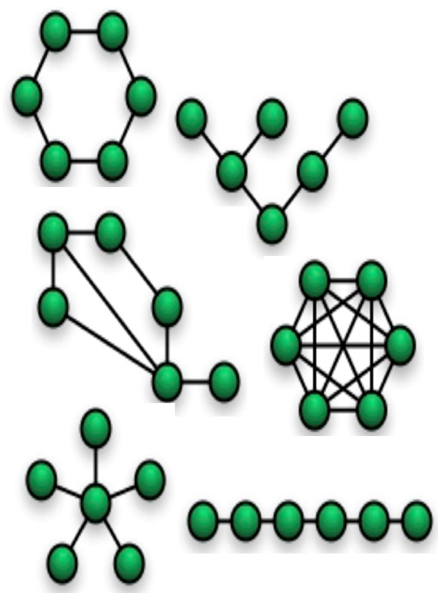


Common Graph Topologies

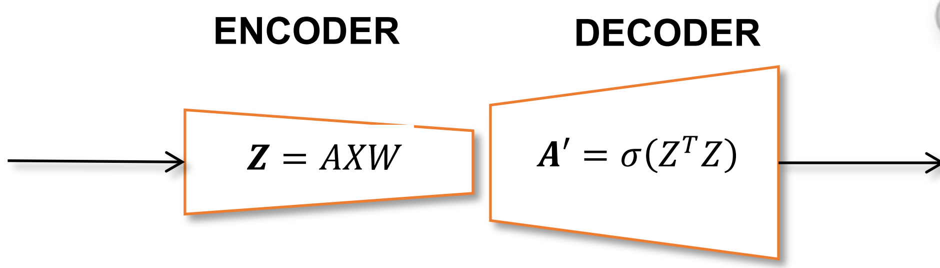
What types of graphs can we auto-encode?

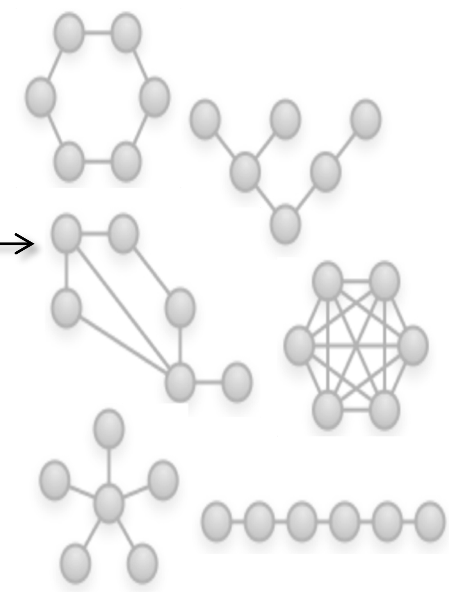


Auto-Encoding Case Studies



Input Graphs



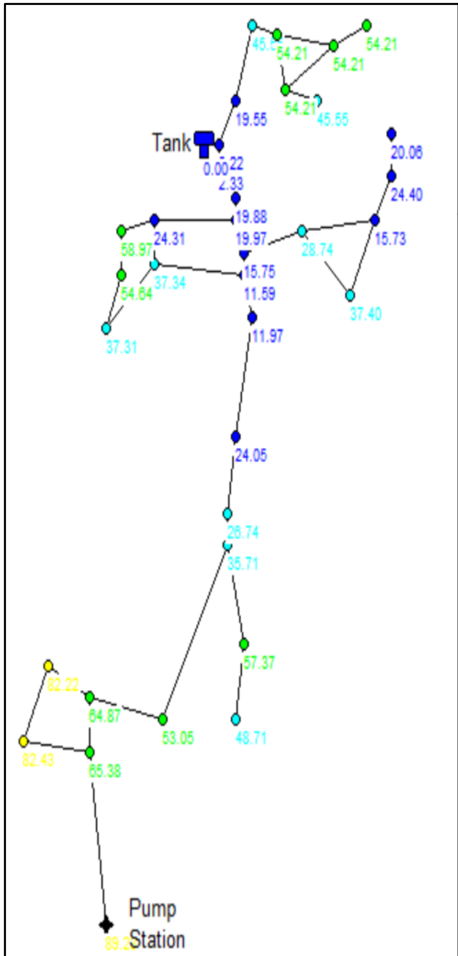


Output Graphs

Graph	No. of Embedding-Layer Neurons Required for Learning
Line	2
Ring	2
Mesh	3
Star	5
Tree	3
FC	1

Mathematical Anomaly

Auto-Encoding an Urban Graph

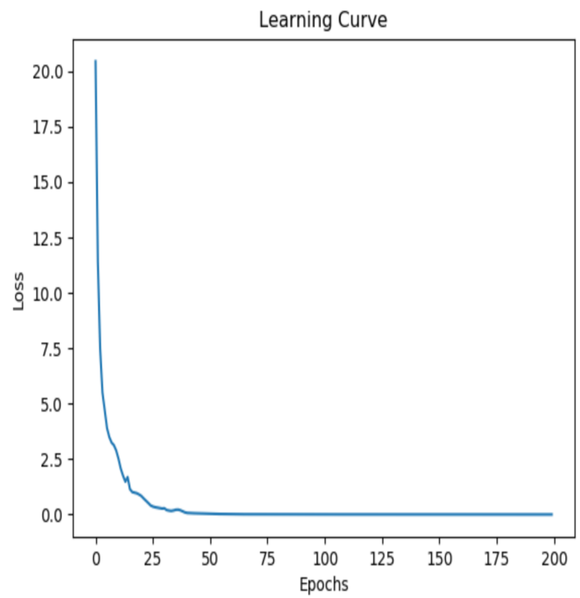


Input Graph

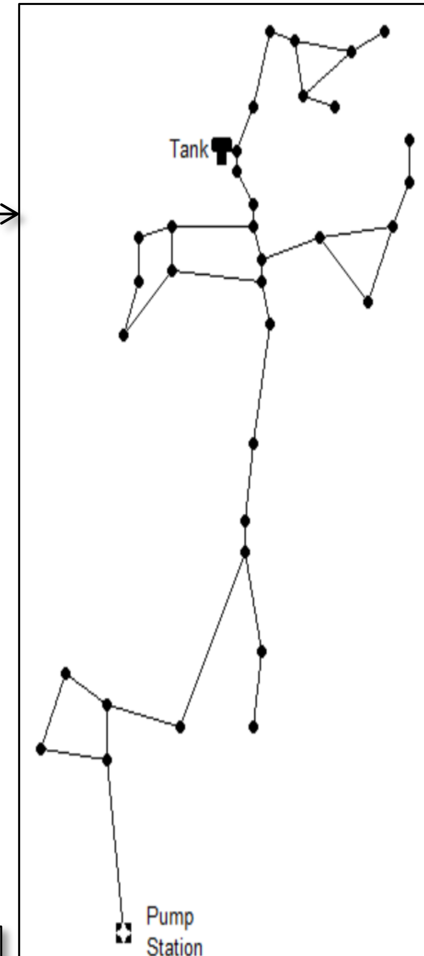
ENCODER **DECODER**

$$\boldsymbol{Z} = AXW$$

$$\boldsymbol{A'} = \sigma(Z^T Z)$$

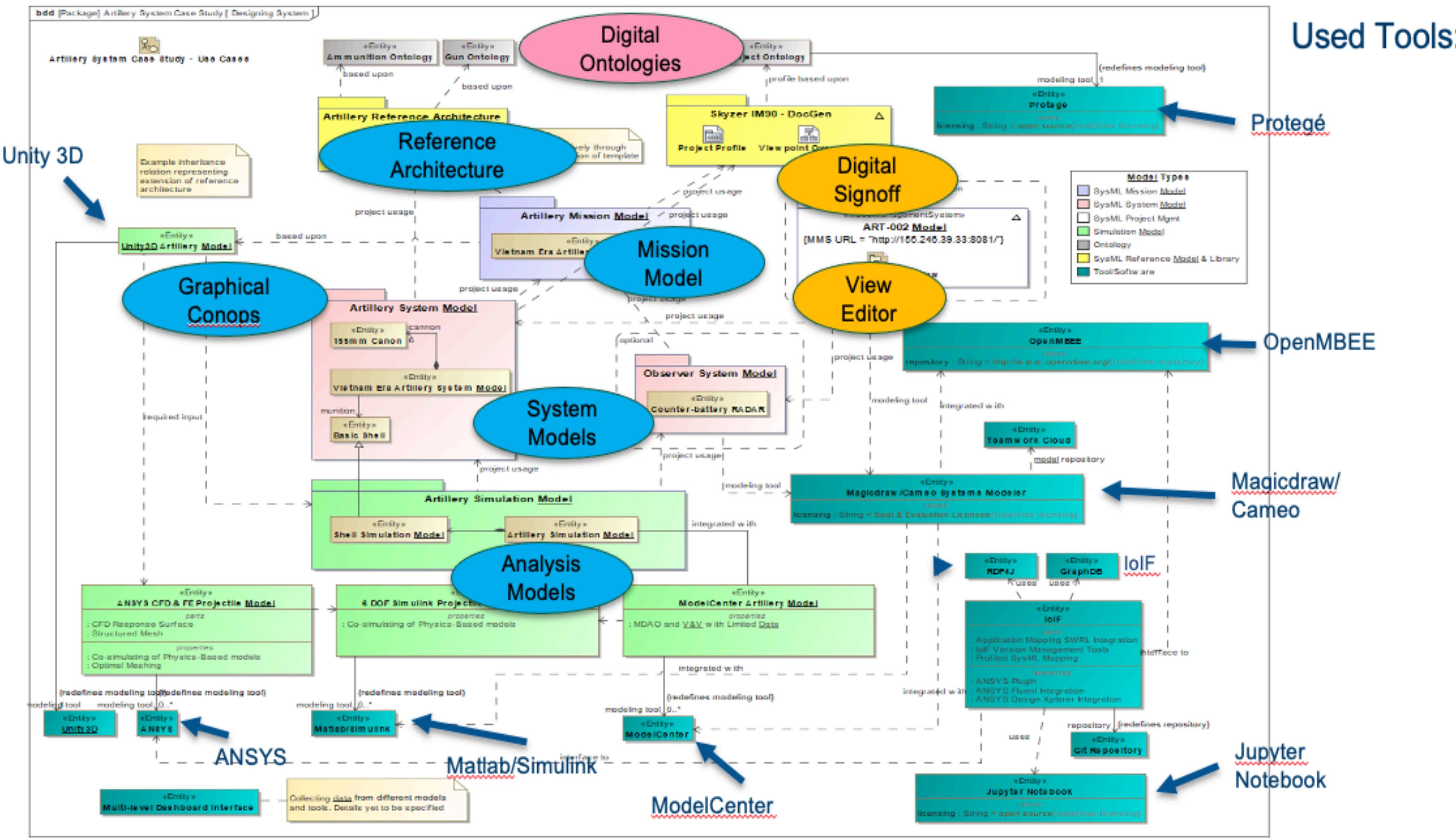


Number of embedding layer neurons = 74
Minimum Loss = 0.00196
Input/Output isomorphism = True



Output Graph

Kind of Data? Semantics with Domain Ontology for "Full Stack" of Models Aligned with Reference Architecture



Distribution Statement A: Approved for public release. Distribution is unlimited.

Future Work

Year 1: Teaching Machines to Understand Graphs

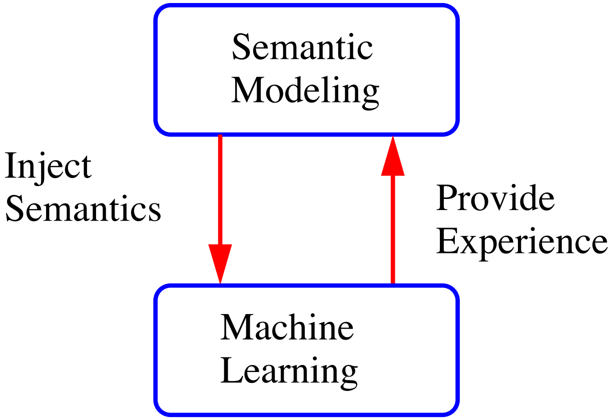
- Teaching machines to understand small graphs having static graph topologies.
- Auto-encoder design (guarantees on system graph representation).
- Formulae for design of neural network architectures for specific types of graph.
- Explore opportunities for composition of neural network architectures.
- Identification of events via time-series anomaly detection.
- Basic mechanisms for semantic / machine learning interaction.
- Integration of simulation and machine learning.

Year 2: Go Deep, Dynamic, Broad, Hybrid

- Deep graph neural networks / dynamic graph topologies.
- Reasoning with events, space and time.
- Inject semantics into machine learning models.
- Applications.

Year 3: Create Digital Twin Experience

- AI/ML architectures for digital twin experience.
- Applications.



Thank You

Questions?

Contact Information

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Mark Blackburn: mblackbu@stevens.edu

References

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- **Coelho M., Austin M.A. and Blackburn M.R.** , Semantic Behavior Modeling and Event-Driven Reasoning for Urban System of Systems, International Journal on Advances in Intelligent Systems, Vol. 10, No 3 and 4, December 2017, pp. 365-382.

- **Coelho M., and Austin M.A.** , Teaching Machines to Understand Urban Networks, The Fifteenth International Conference on Systems (ICONS 2020), Lisbon, Portugal, February 23-27, 2020, pp. 37-42.

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- **Coelho M., Austin M.A., and Blackburn M.R.,** The Data-Ontology-Rule Footing: A Building Block for Knowledge-Based Development and Event-Driven Execution of Multi-Domain Systems, 2018 Conference on Systems Engineering Research, Charlottsville, VA, May 8-9, 2018. Also see: Chapter 21, Systems Engineering in Context , Springer, 2019.

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Extra Slides

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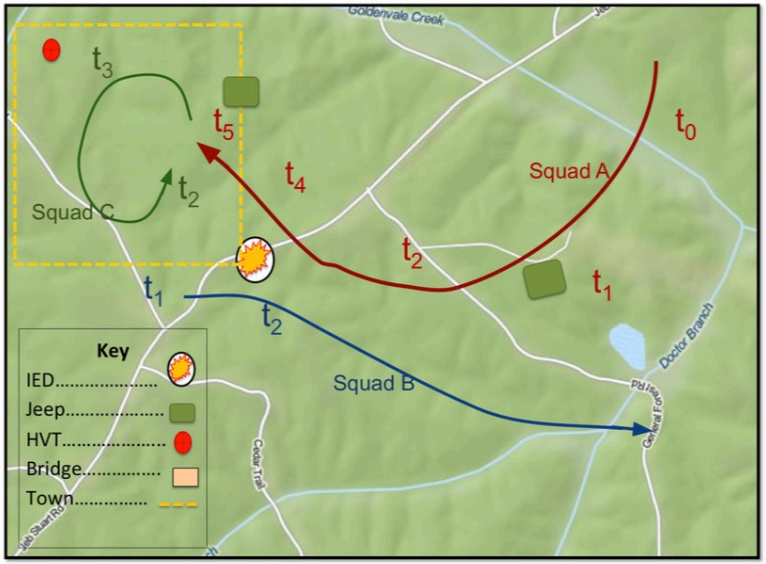
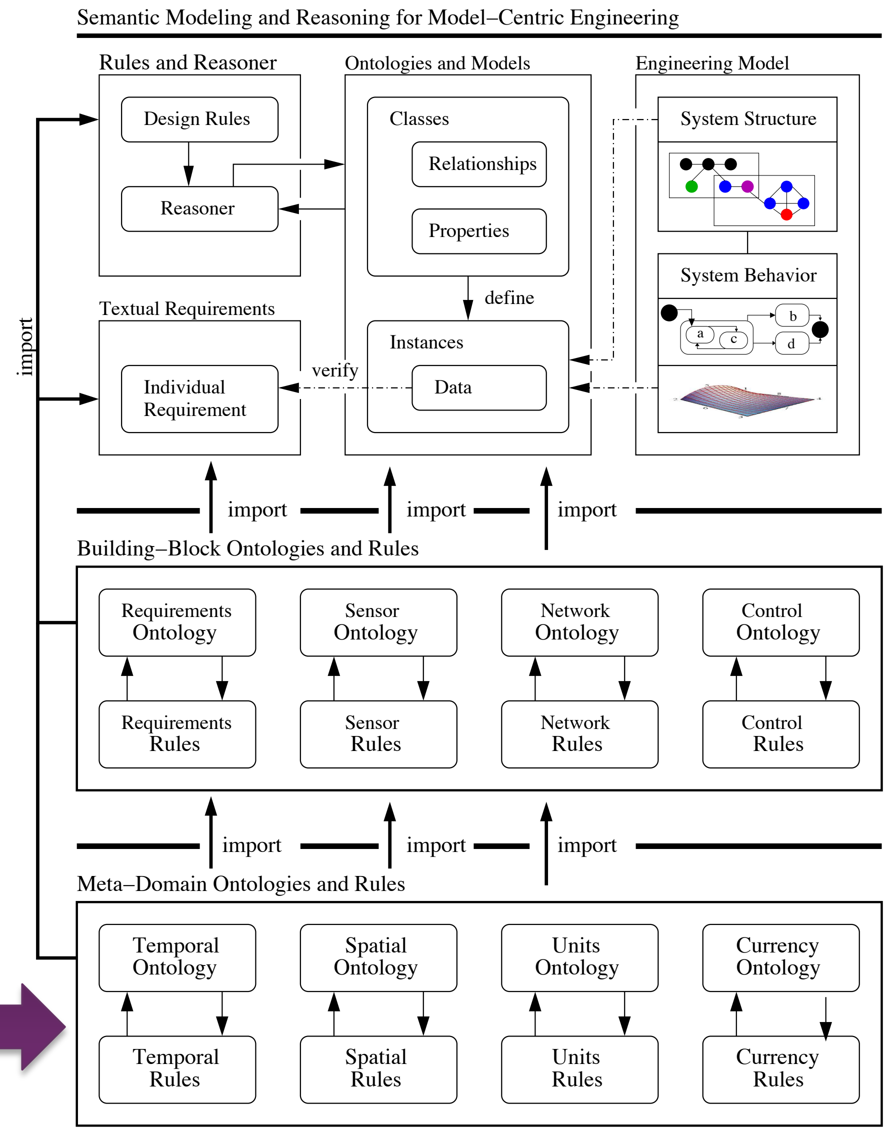
Semantic Modeling for Model-Centric Engineering

Simple Military Exercise



Decision Making / Exercise Actions

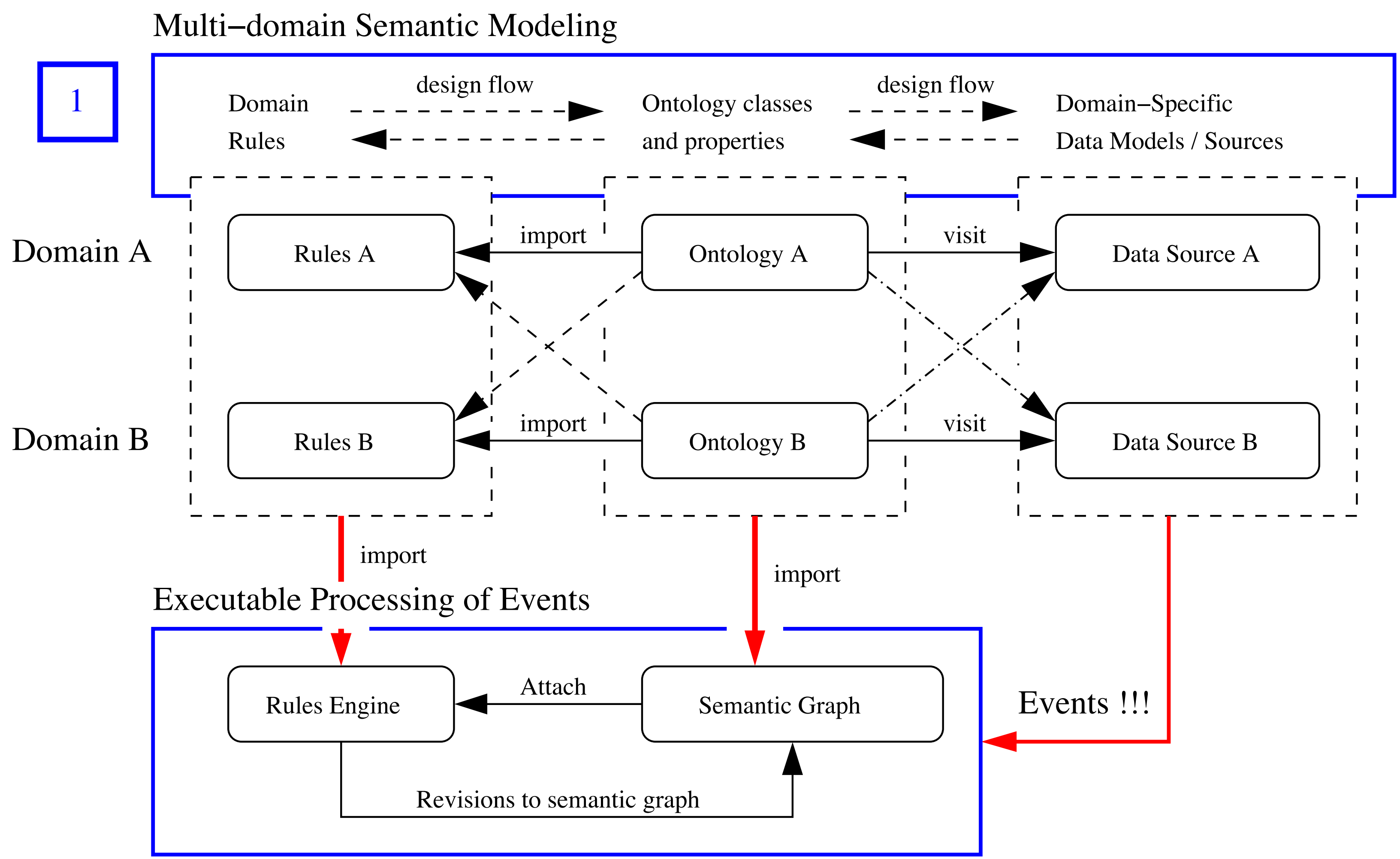
Military exercise actions need to occur at the right time and in the right place.



Source: Regli W., et al.

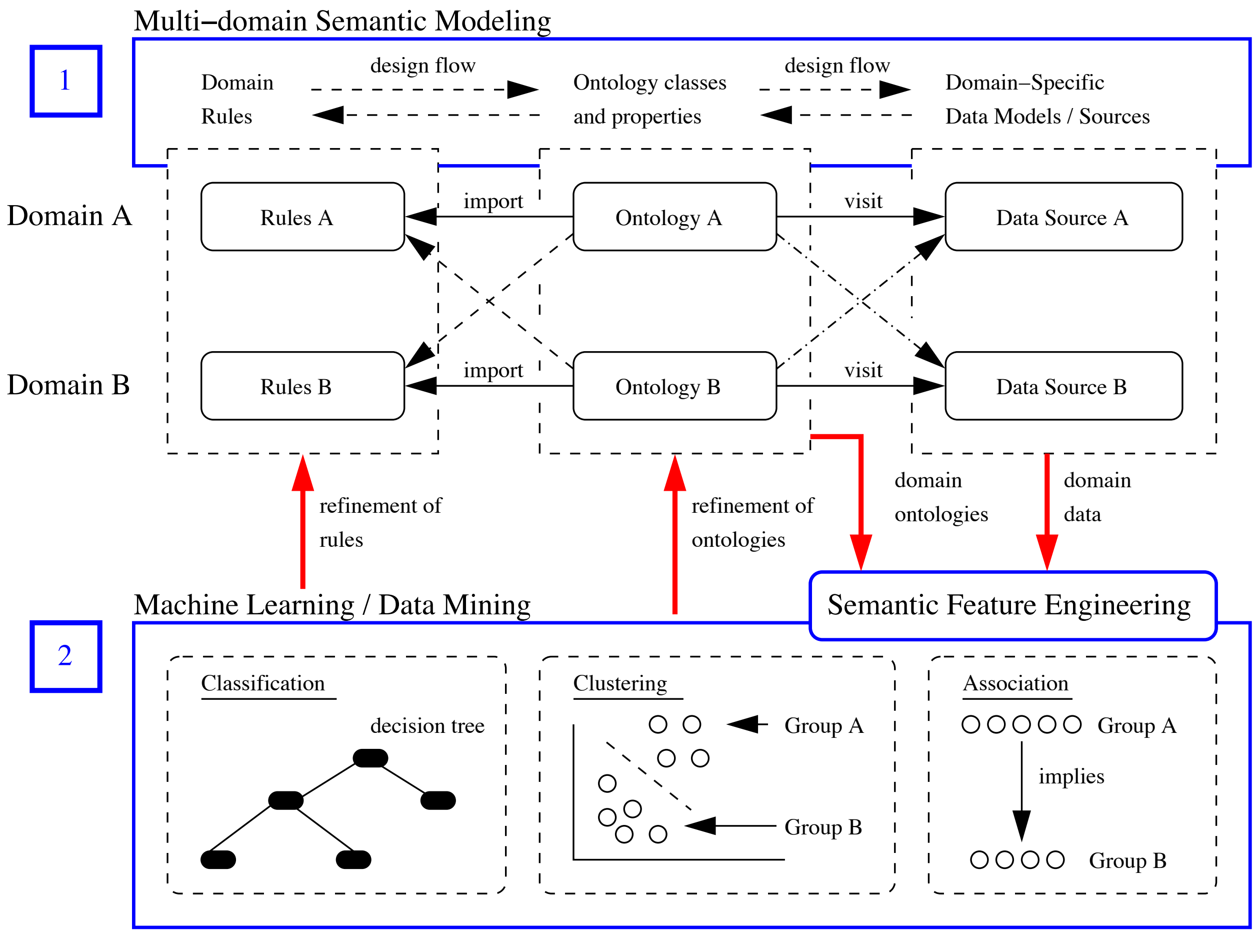
Multi-Domain Semantic Modeling

Data-Ontology-Rule Footing (Work at UMD / NIST / SERC in 2017).



Combined Semantics + Data Mining

Work at UMD / Building Energy Group at NIST / NCI, 2018-2019



Research Question: How can semantic modeling + machine learning / data mining work together as a team?