

Universal Systems Simulation via Constraint Hypergraphs with Applications to Digital Twins

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6 November 2025

PhD Defense

Dept. of Mechanical Engineering | Clemson University



Biographical Sketch

(2018) Married

BS: Mech Engr, BYU (2021)



(2021) Started as PLM Applications Engineer

Birth of first son (2021)

(2023) Birth of second son

MS: Mech Engr, Clemson (2023)



(2024) Collaboration with NPS

Visiting Researcher at NIST (2025)



(2025) Birth of third son

PhD: Mech Engr, Clemson (2025)



(2026) Collaboration with Alan Turing Institute

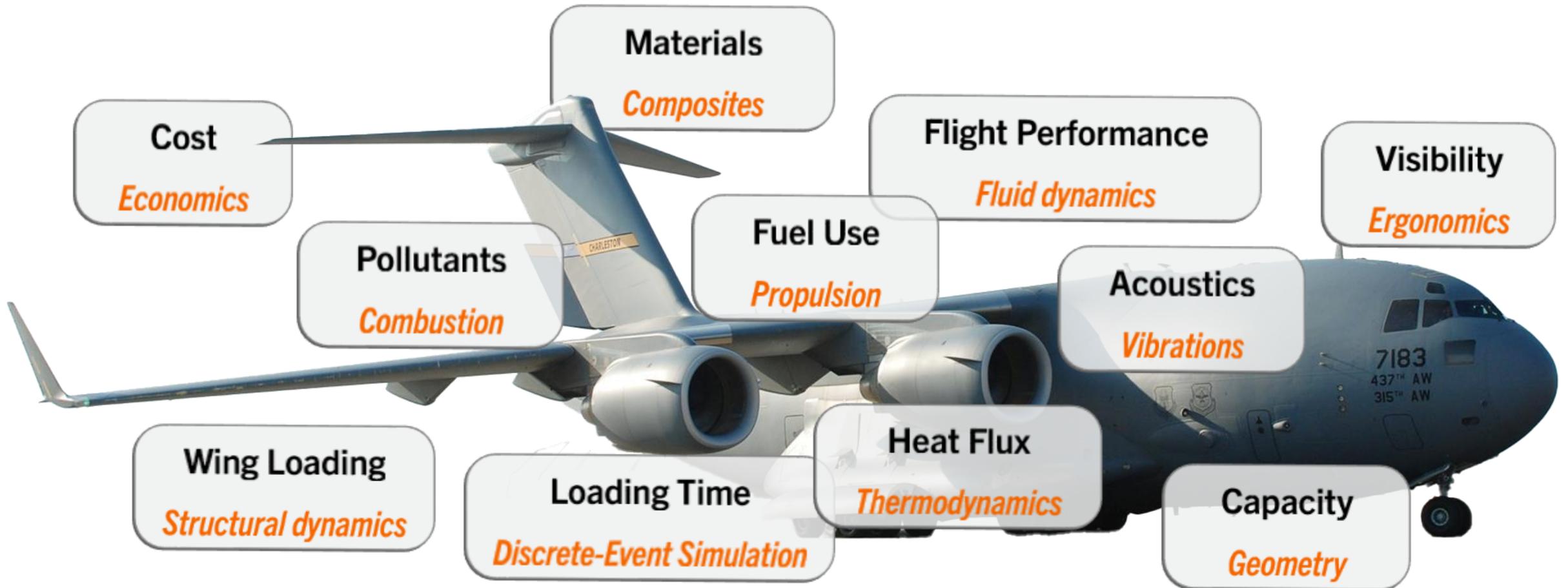
Post-doctoral fellowship with NPS (2026)



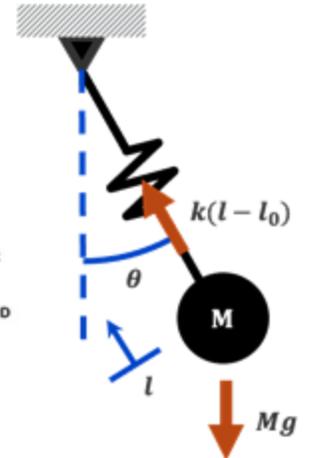
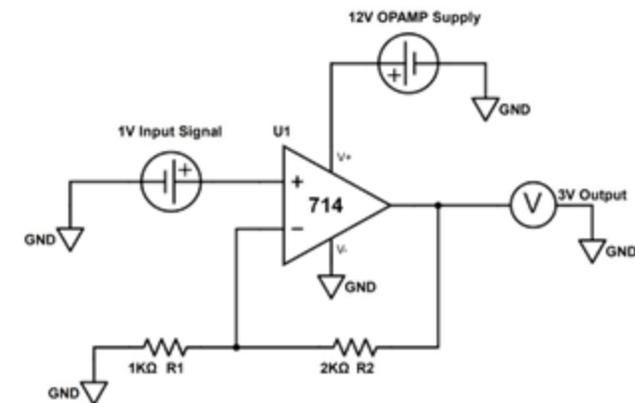
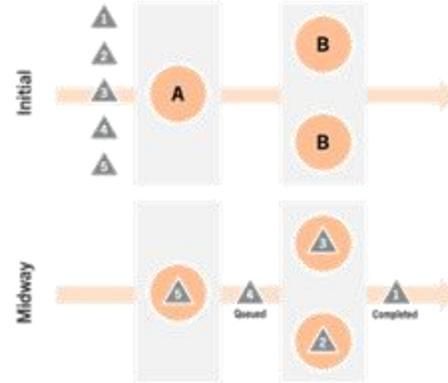
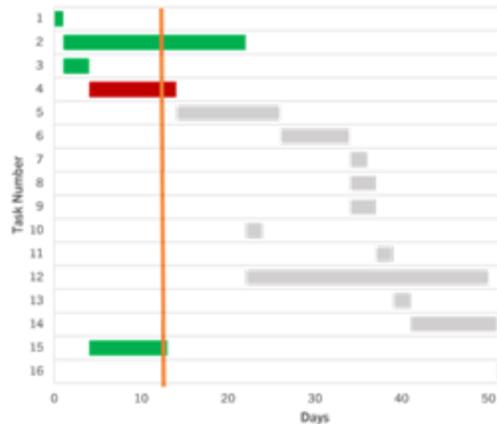
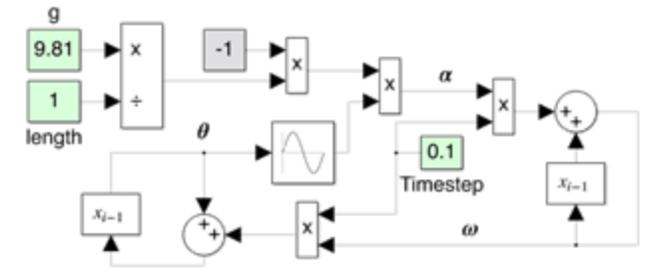
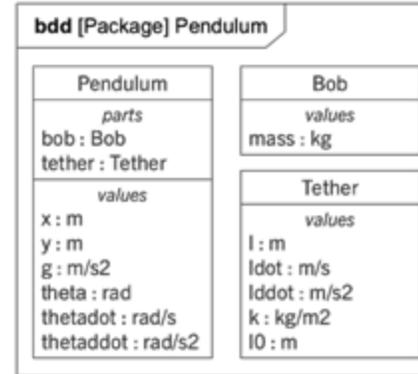
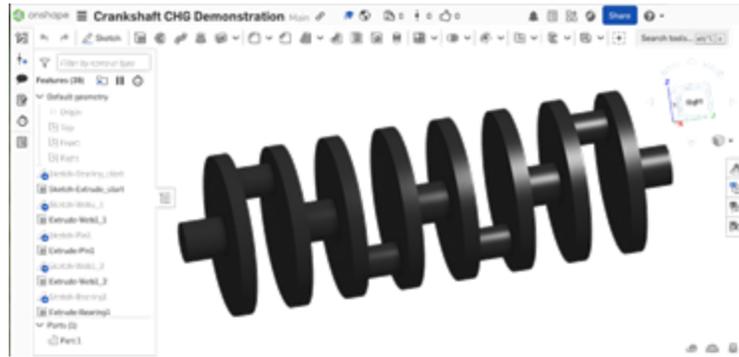
Science is the work of describing the worlds around us



Knowing information about complex systems require models across many domains

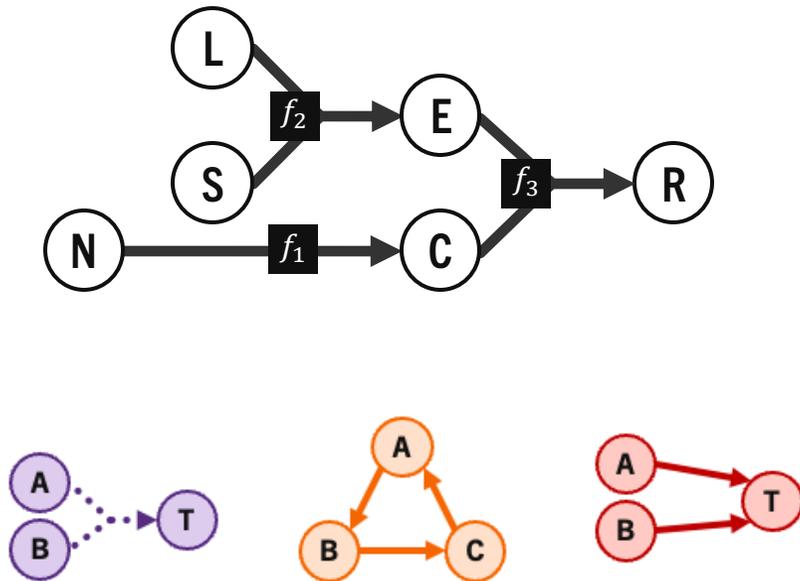


Most modeling frameworks have limited universality and descriptiveness

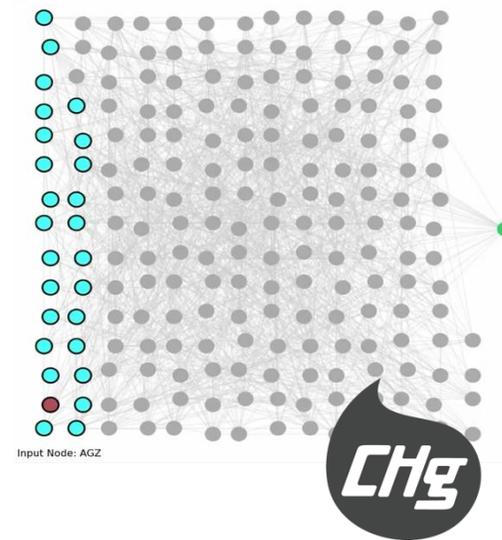


Constraint hypergraphs are a framework for universal, declarative systems modeling

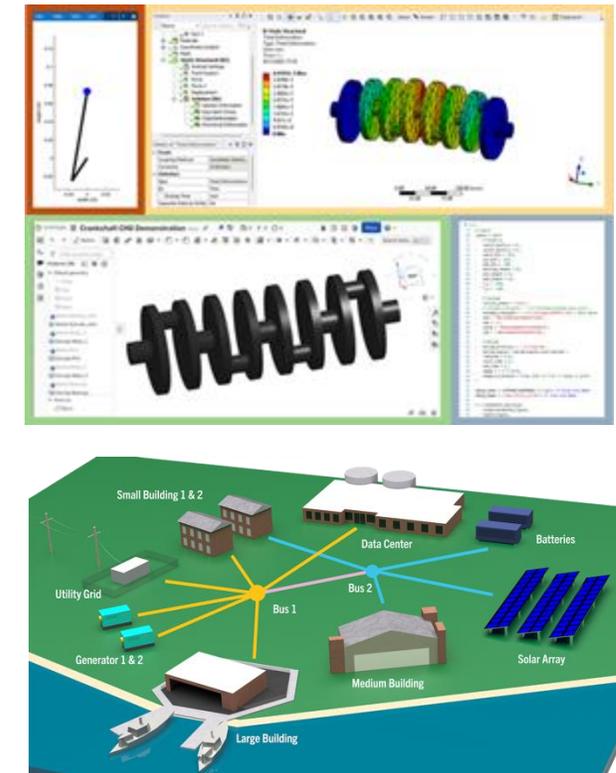
CHG Definition



Declarative Simulation



Applications



Introduction to CHGs

Universal System Simulation via Constraint Hypergraphs

Information is what we can distinguish about a system

Economy (L/km)

Color



Fuel Capacity (L)

Name

“A system is a collection of variables” –Ross Ashby

A state is data that must be temporally consistent

Economy (L/km)

10

11

12

Color

Blue

Gray

Tan

Fuel Capacity (L)

100,000

115,000

130,000

Name

C-17 Globemaster

C-5 Galaxy

C-130 Hercules



We describe systems by either observations or simulations

Economy (L/km)

10

11

12

Color

Blue

Gray

Tan

Fuel Capacity (L)

100,000

115,000

130,000

Name

C-17 Globemaster

C-5 Galaxy

C-130 Hercules



Observations are measurements we make of reality

Economy (L/km)

10

11

12

Color

Blue

Gray

Tan

Fuel Capacity (L)

100,000

115,000

130,000

Name

C-17 Globemaster

C-5 Galaxy

C-130 Hercules



Simulations are predictions we make based on relationships



Economy (L/km)
10
11
12

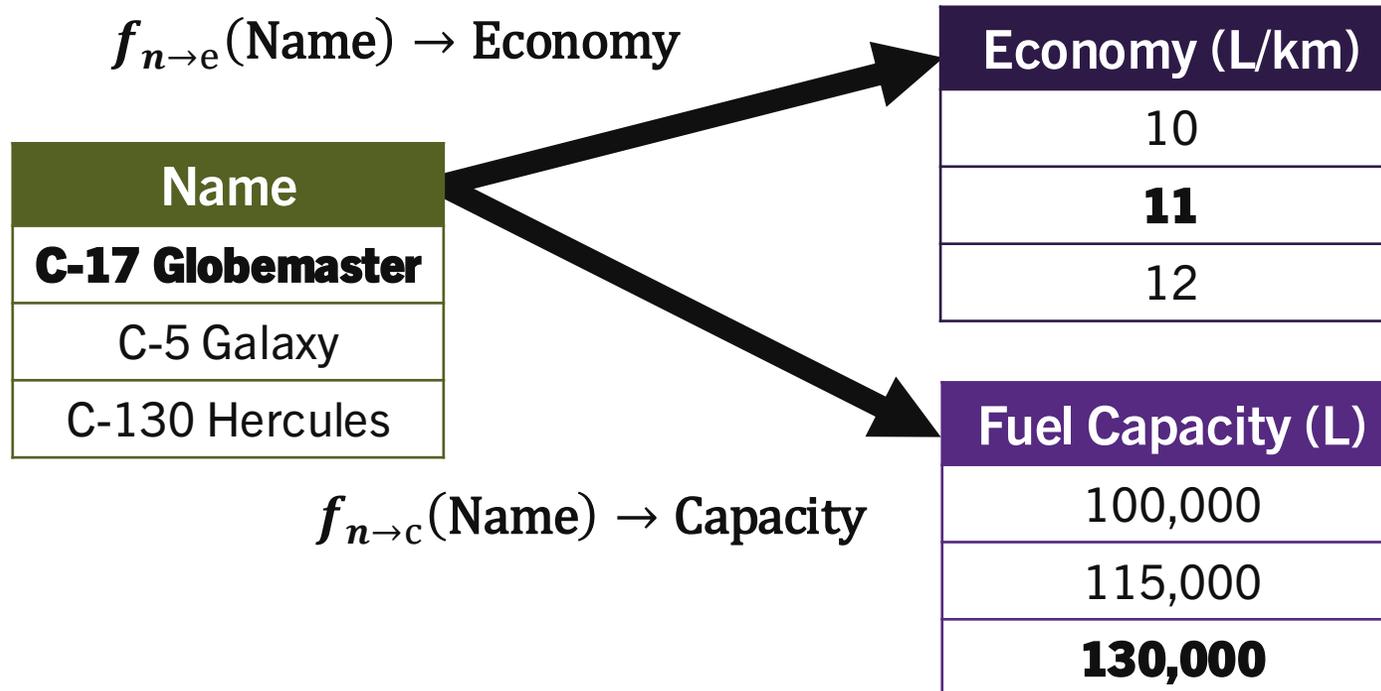
Color
Blue
Gray
Tan

Fuel Capacity (L)
100,000
115,000
130,000

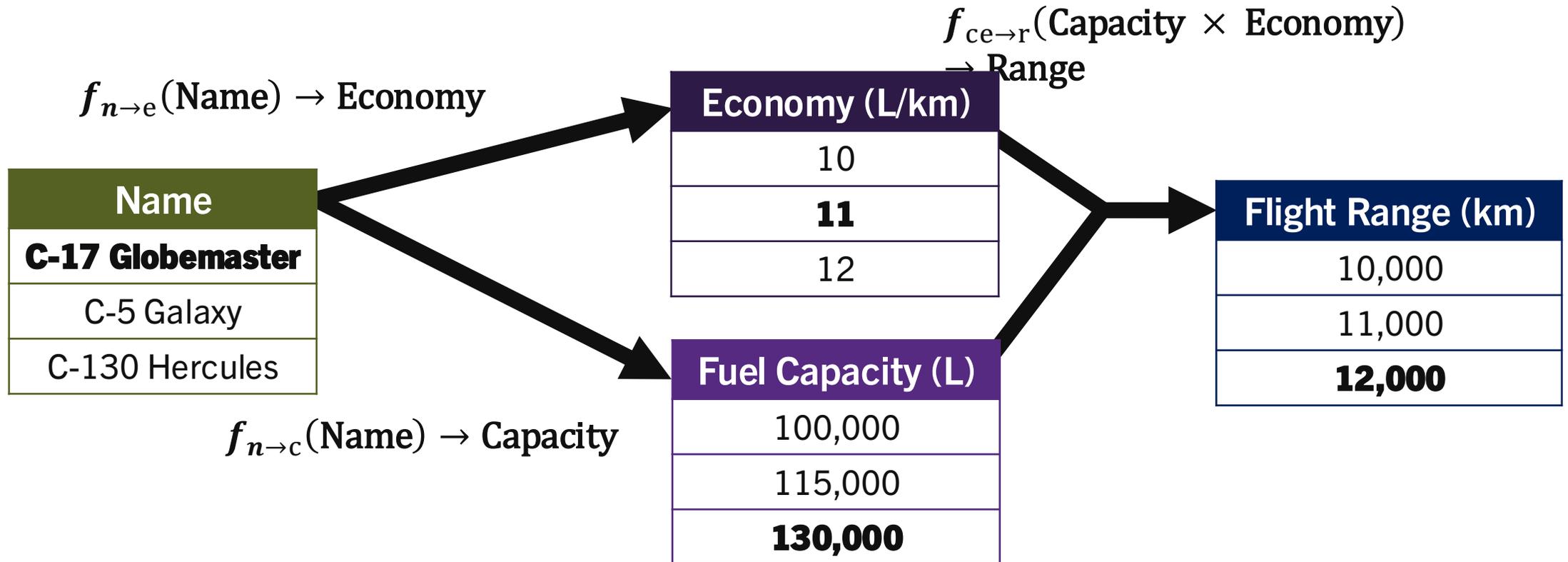
Name
C-17 Globemaster
C-5 Galaxy
C-130 Hercules

(Database lookup)

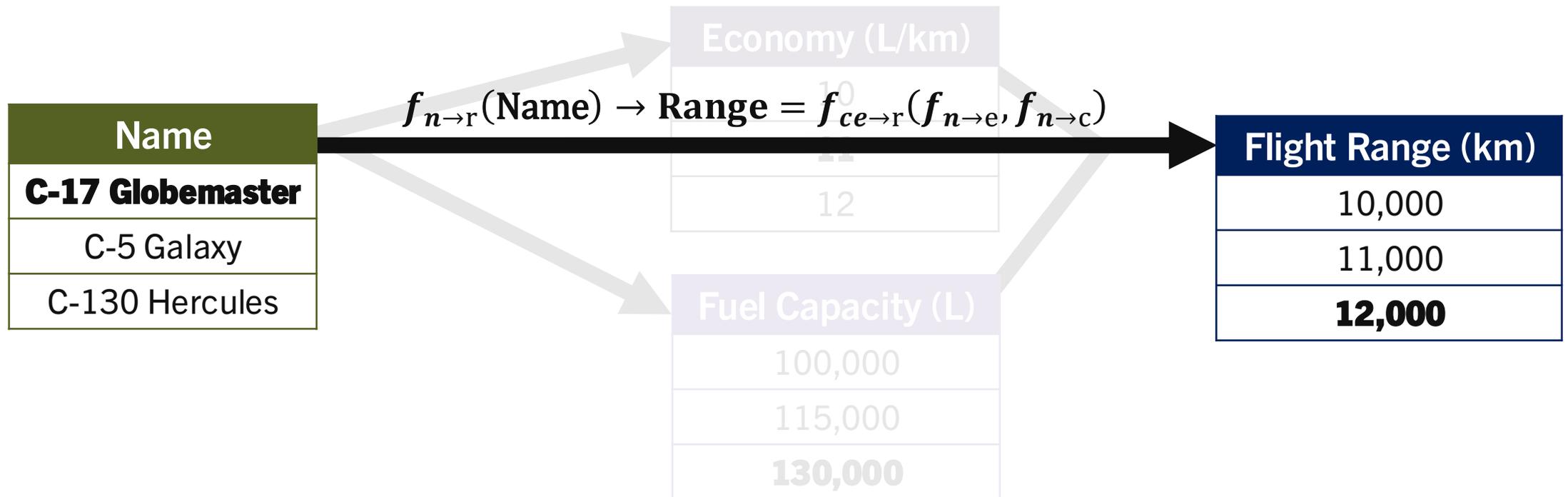
Model relations are algebraic functions that describe behavior



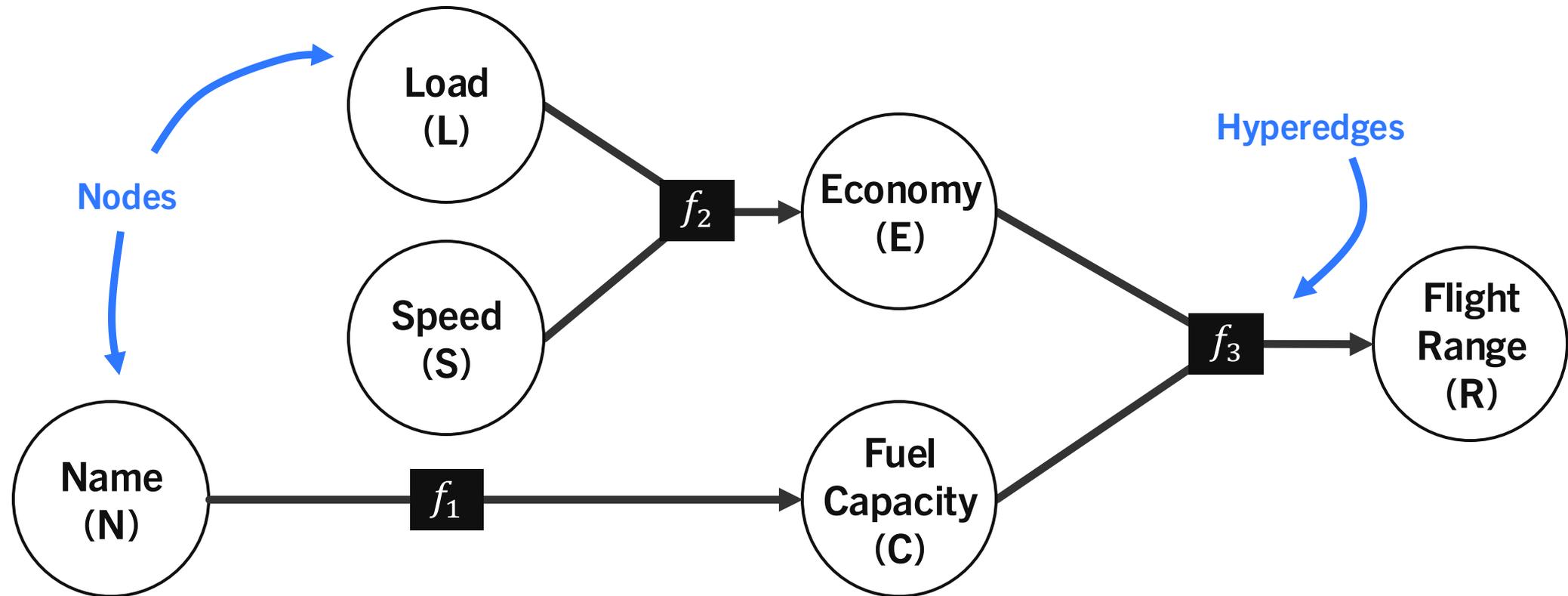
Functions can have multiple arguments



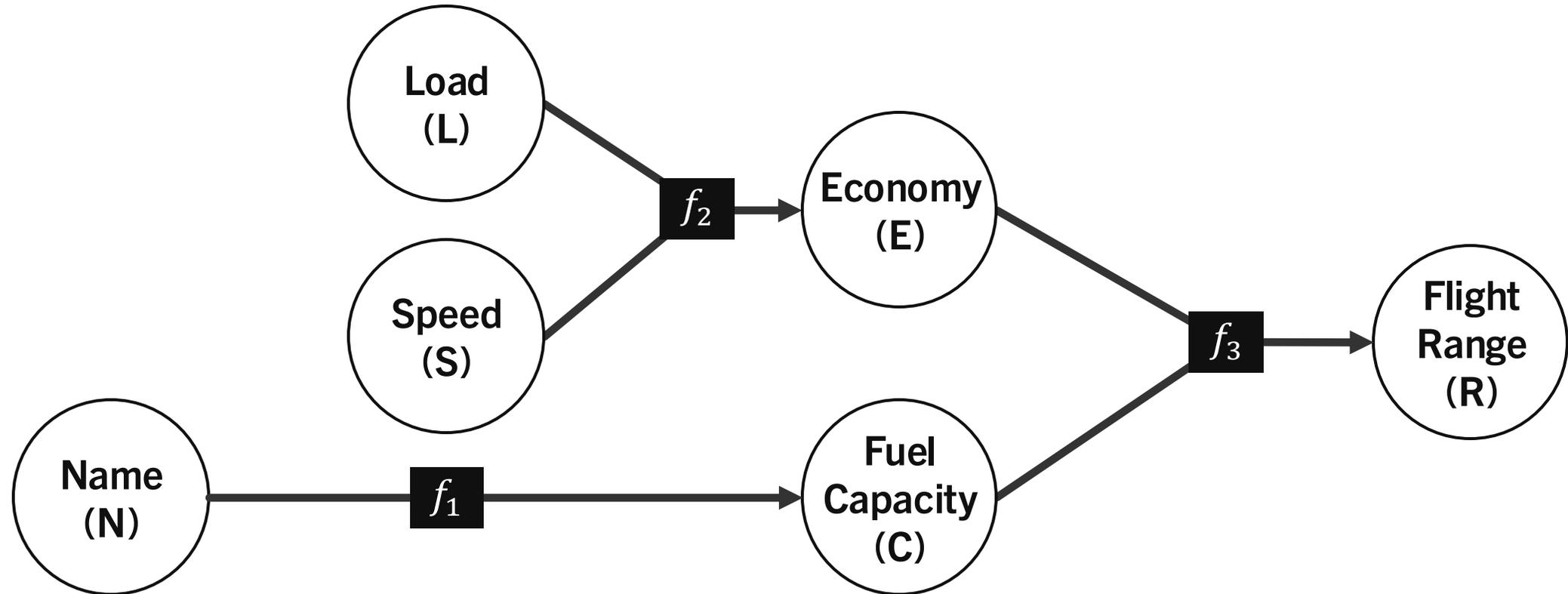
Functions compose to form greater functions



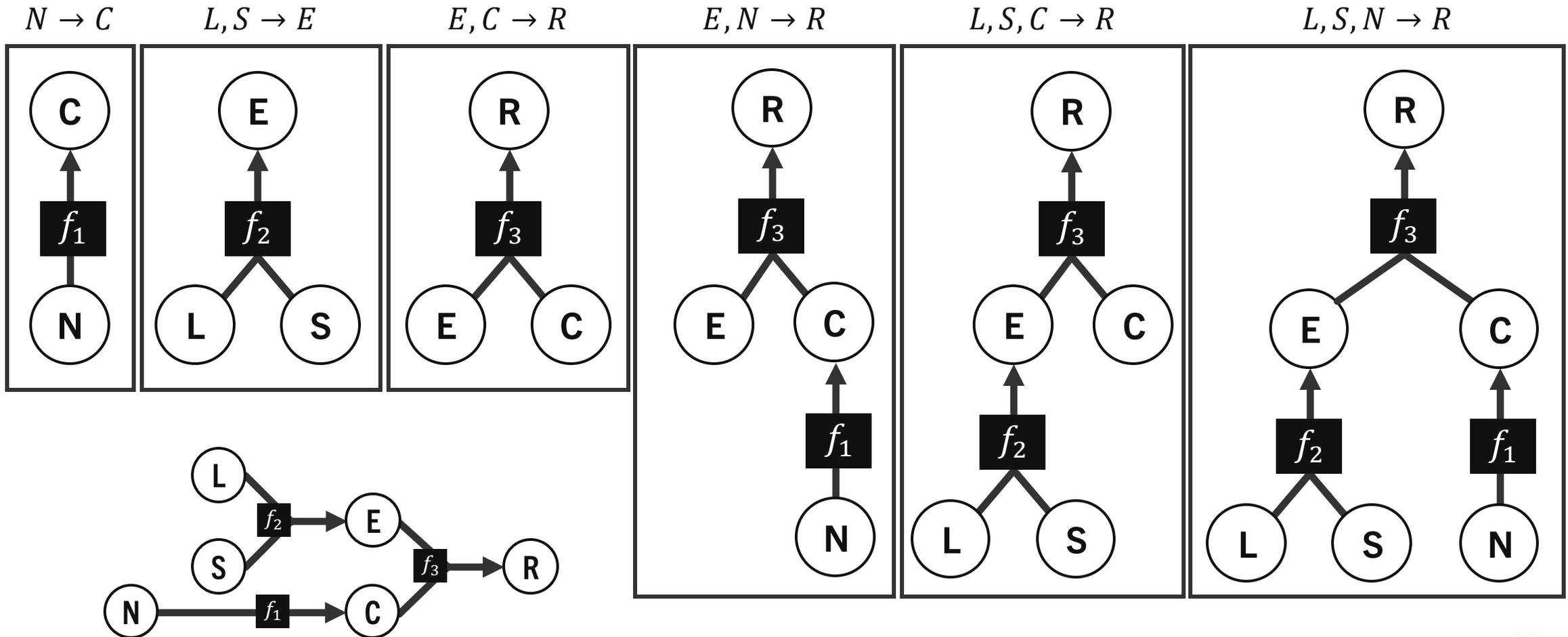
We can represent all models and variables as a constraint hypergraph (CHG)



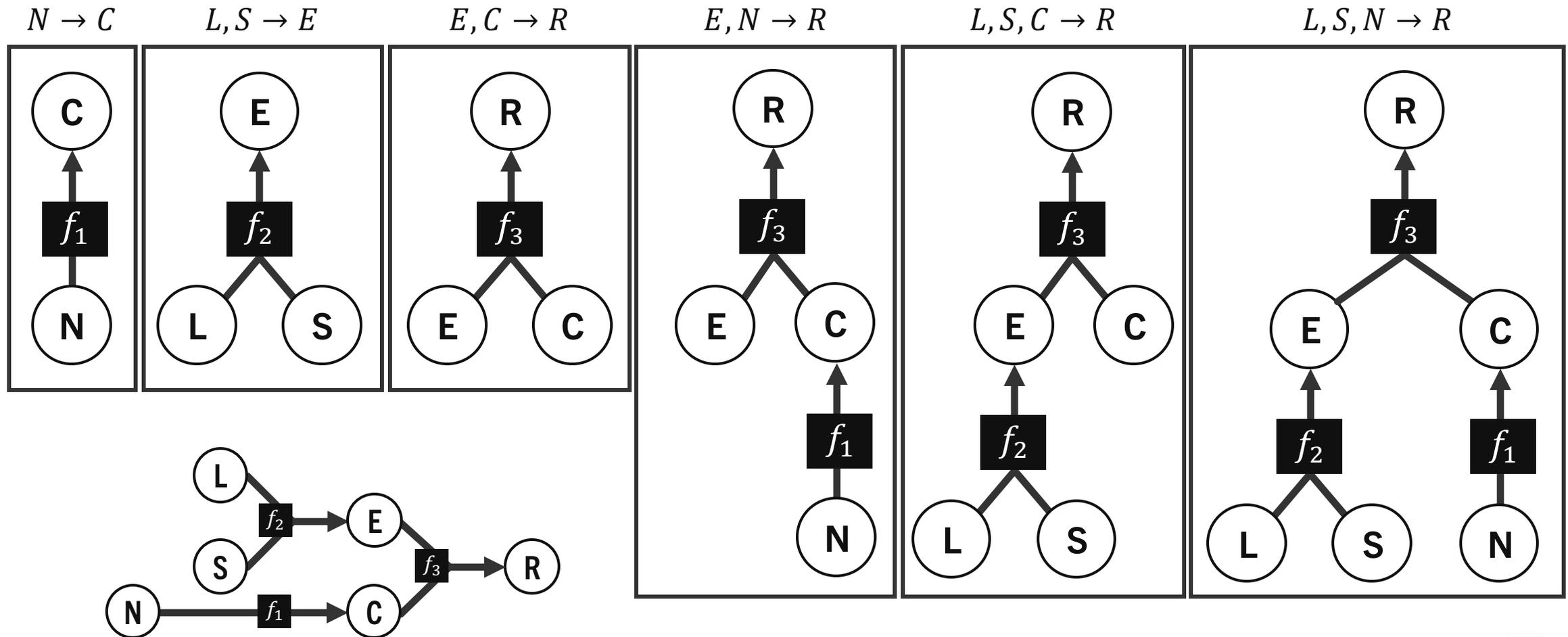
Every path in a CHG is a simulation



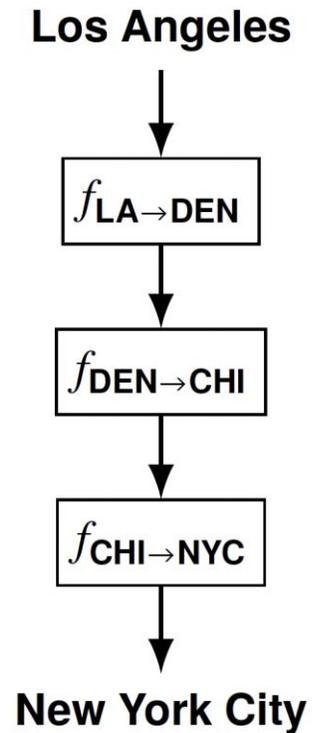
Every path in a CHG is a simulation



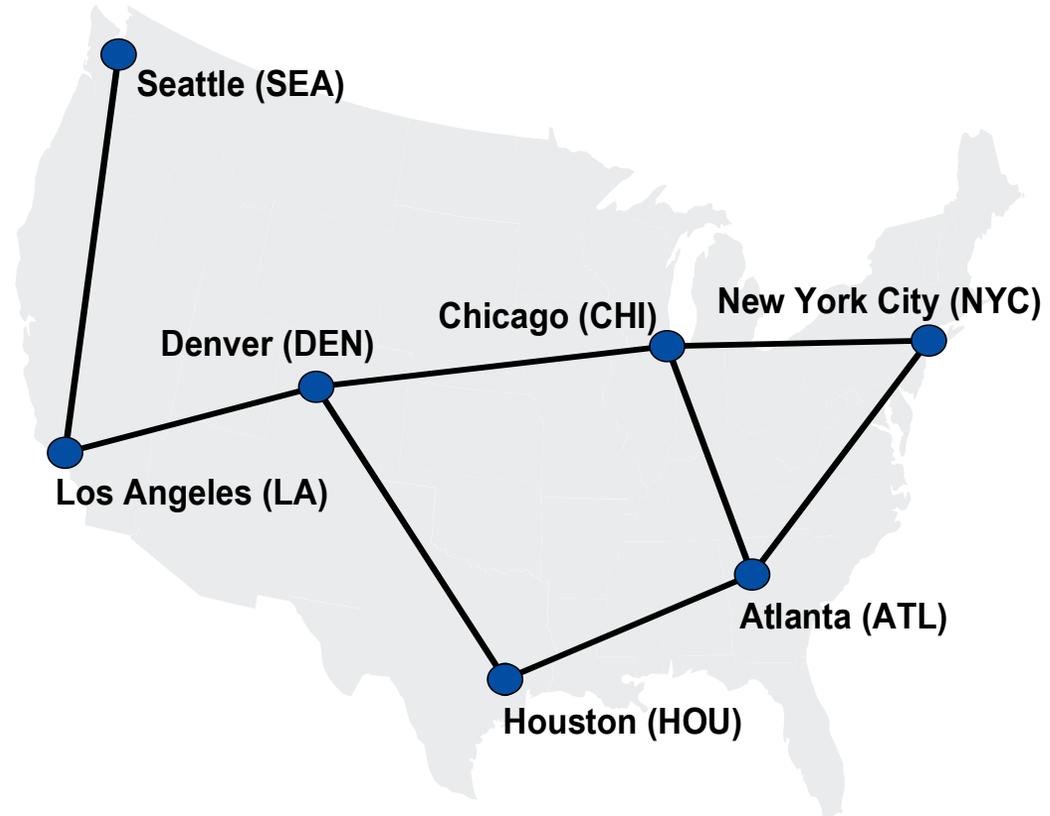
Embedded behavior (paths) enables declarative simulation



Declarative models capture the semantics of the system

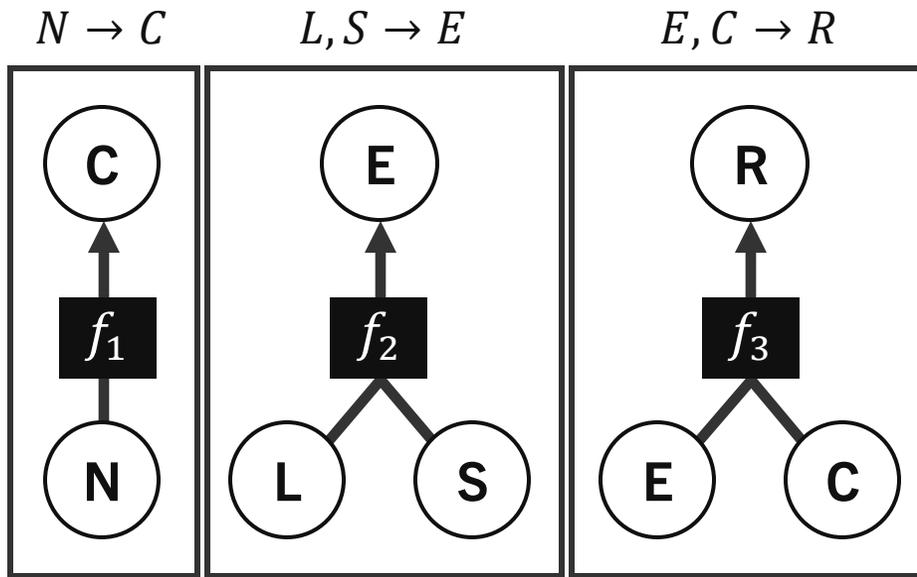


Imperative

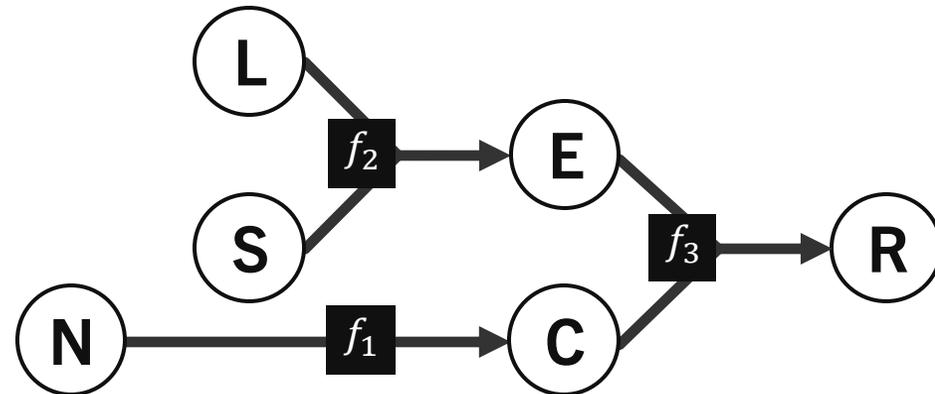


Declarative

Declarative simulation in a CHGs is pathfinding

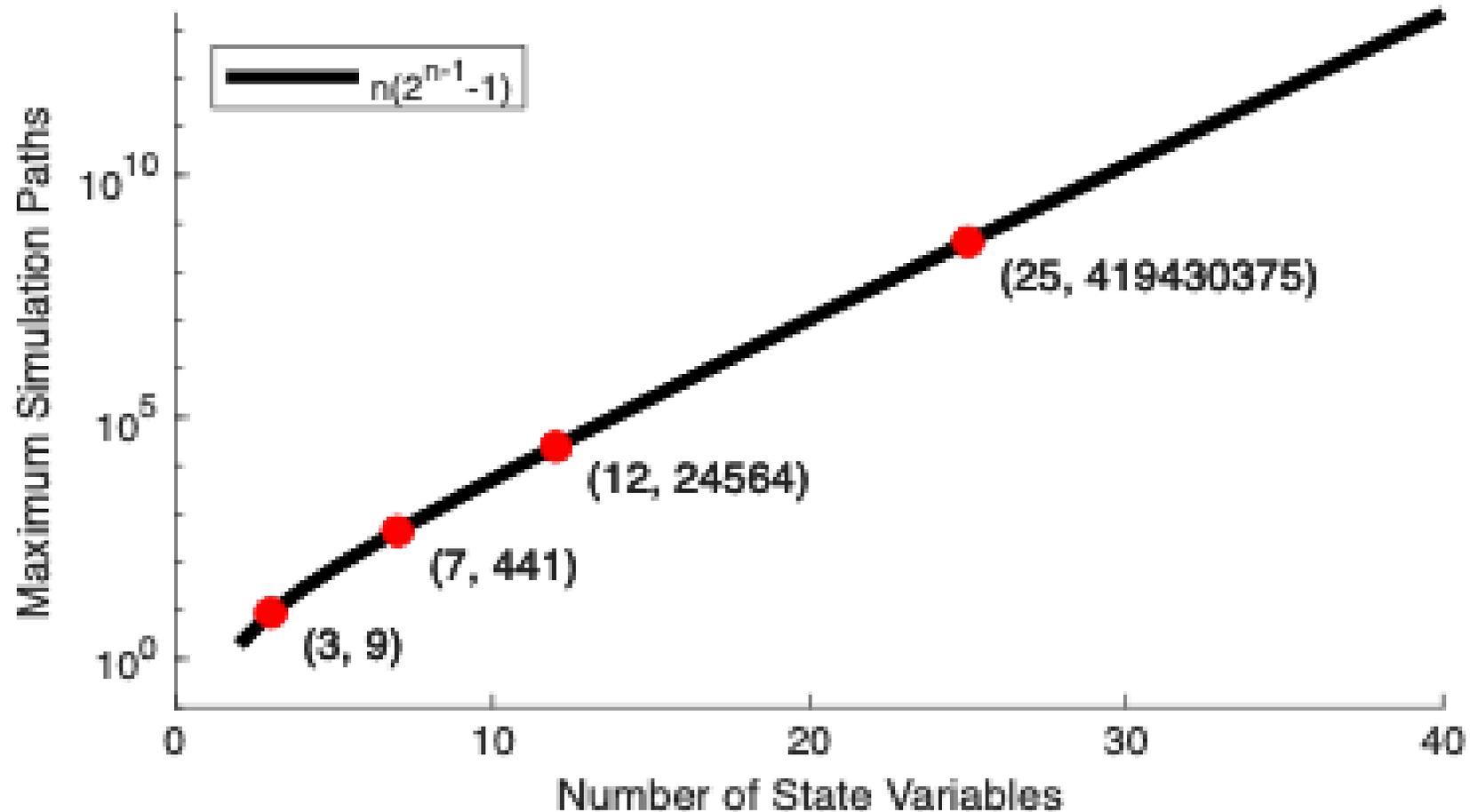


Imperative



Declarative

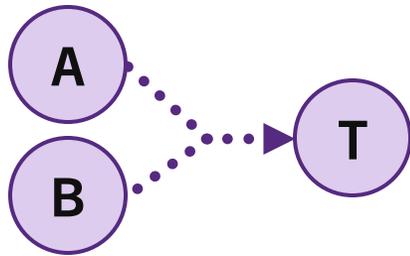
CHGs reduce complexity of expressing simulation paths



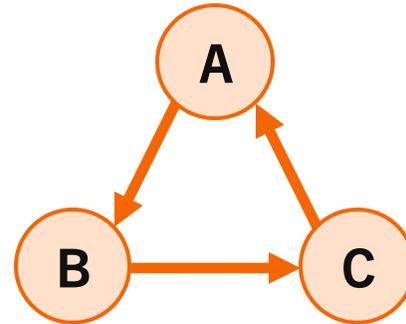
Structure of a CHG

Universal System Simulation via Constraint Hypergraphs

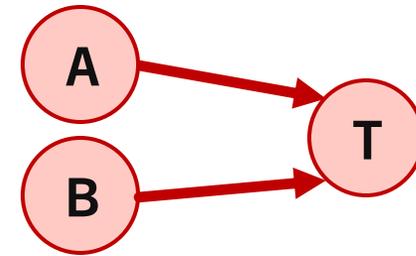
There are three structures in a CHG that a declarative agent needs to process:



Partial Edges

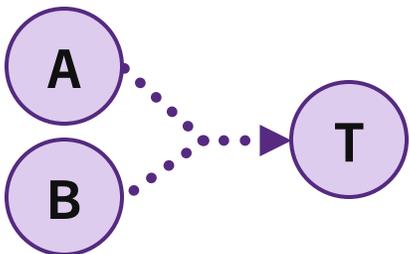
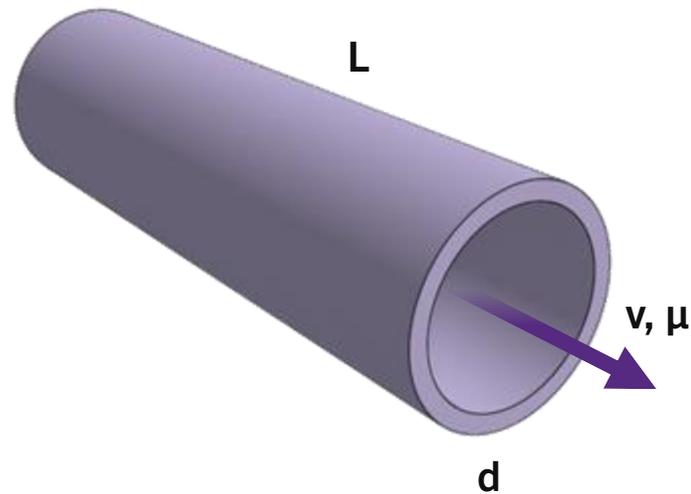


Cycles



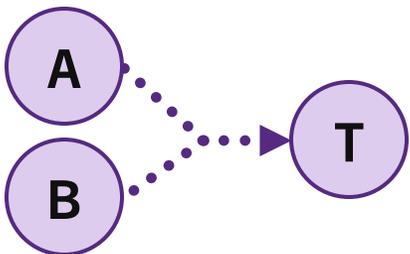
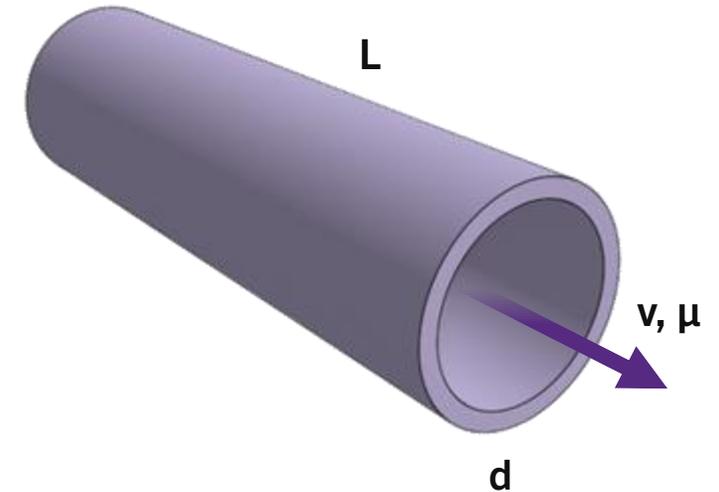
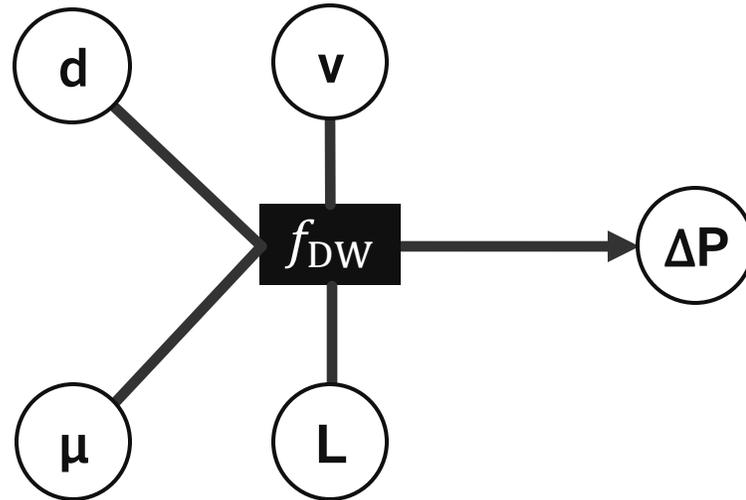
Multi-Edges

Partial edges occur when we don't have an explicit mapping for every variable



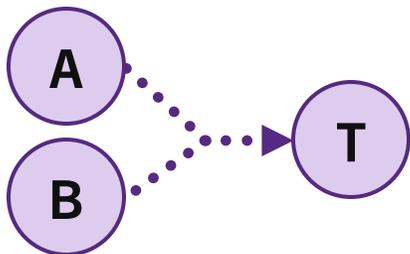
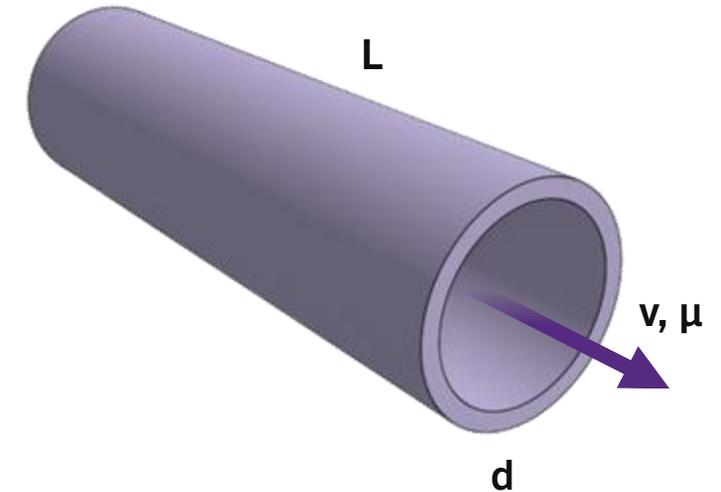
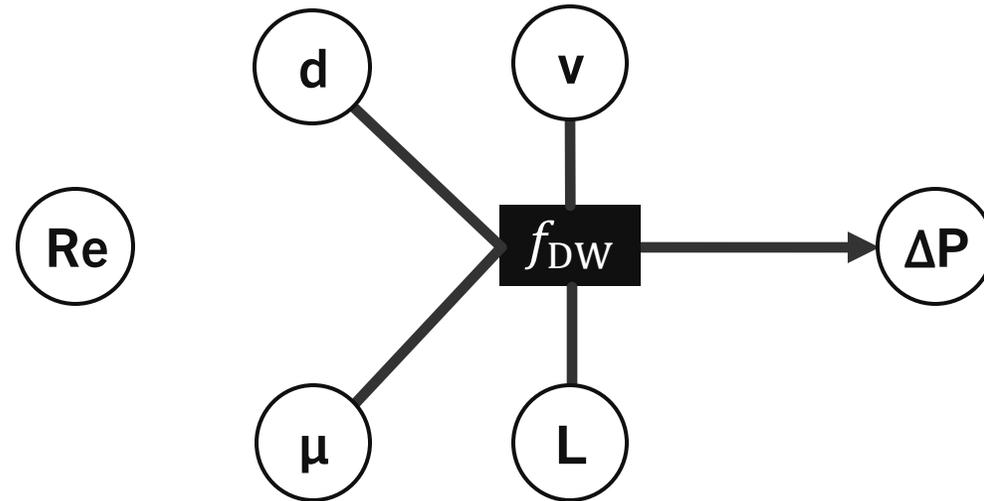
Goal is to calculate pressure loss from fluid flow in a pipe

Partial edges occur when we don't have an explicit mapping for every variable



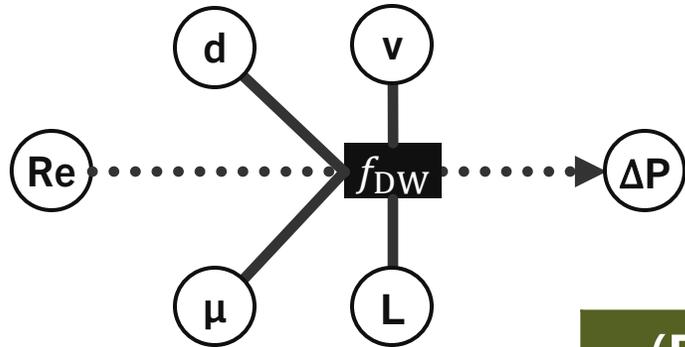
The hypergraph captures the Darcy-Weisbach relationship $\Delta P = \frac{32\mu v L}{d^2}$

Partial edges occur when we don't have an explicit mapping for every variable

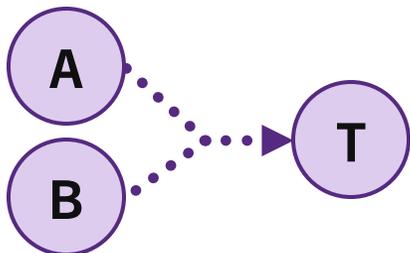
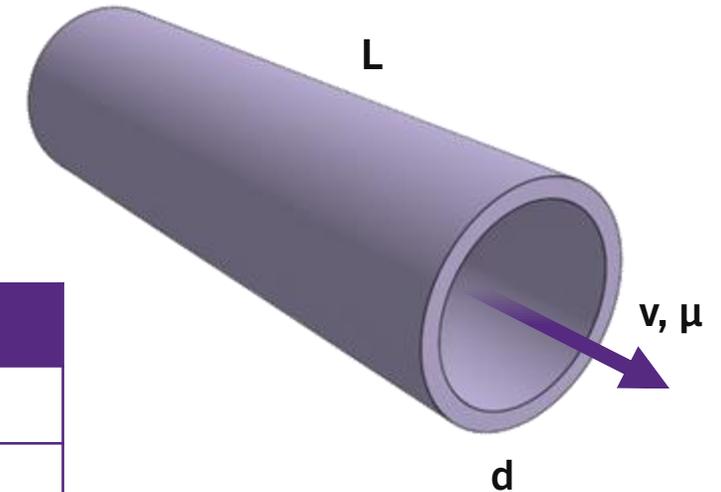


This relationship is only valid if the flow is laminar ($Re < 2300$)

Partial edges occur when we don't have an explicit mapping for every variable

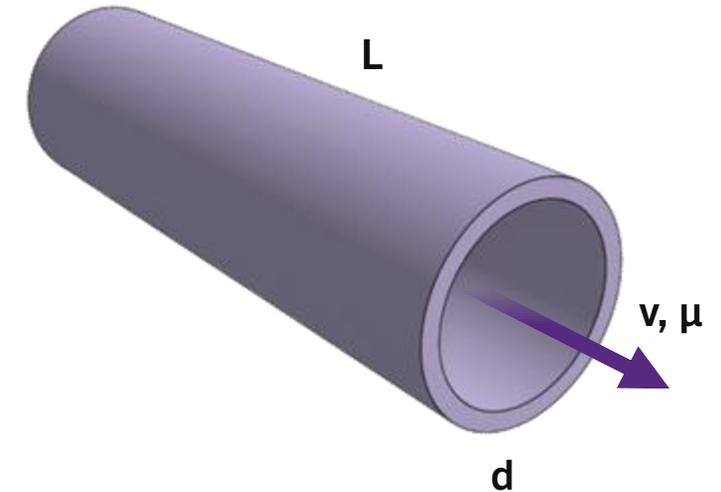
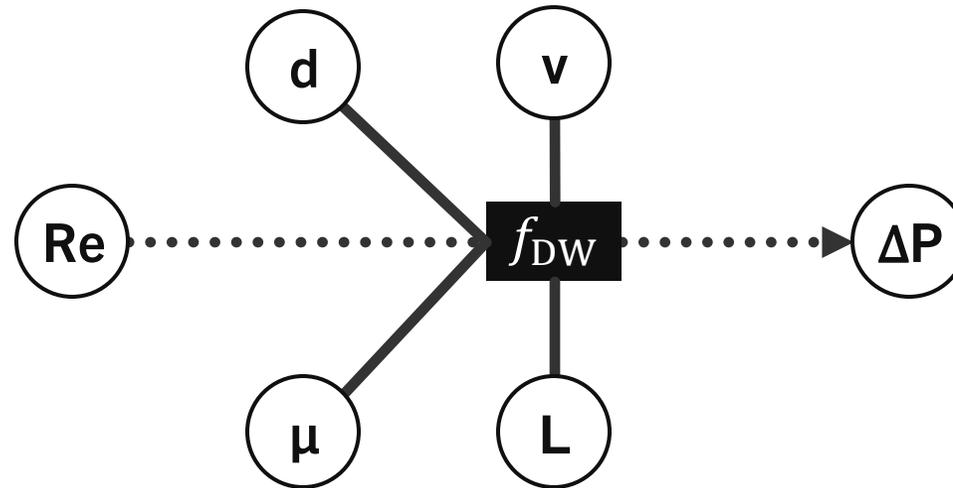
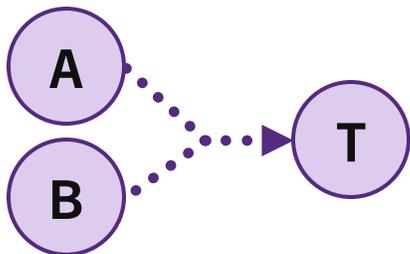


(Re, L, μ, d, v)	f_{DW}	ΔP
...		...
$(1000, L, \mu, d, v)$	→	0.5
$(2000, L, \mu, d, v)$	→	1
$(3000, L, \mu, d, v)$		1.5
...		...



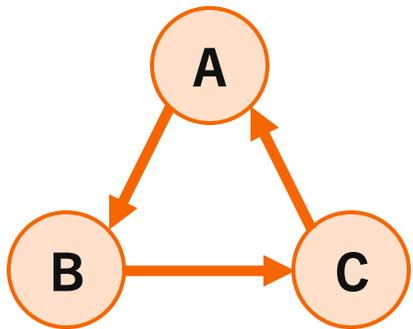
We show this by mapping a subset of the domain

Partiality means that functions don't automatically compose



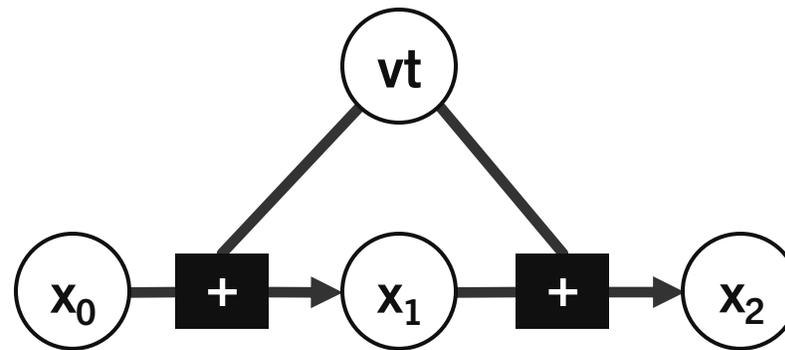
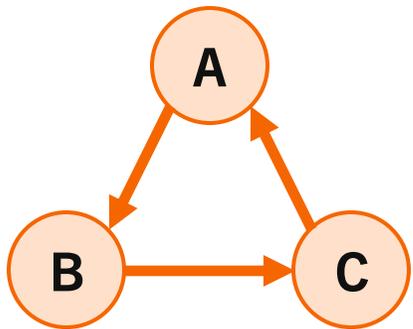
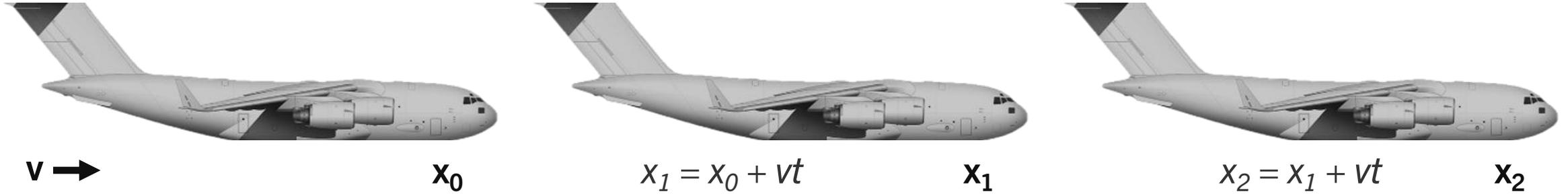
The dotted line shows that our function doesn't handle every value of Re

Cycles indicate behavioral patterns



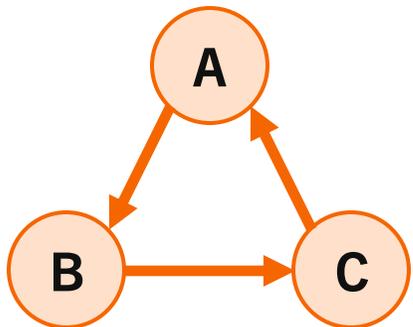
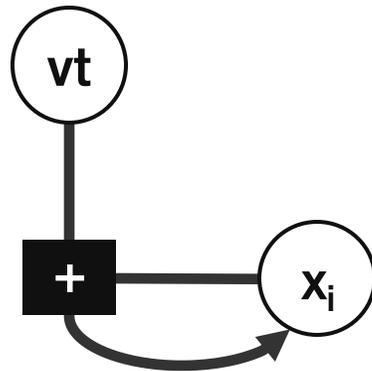
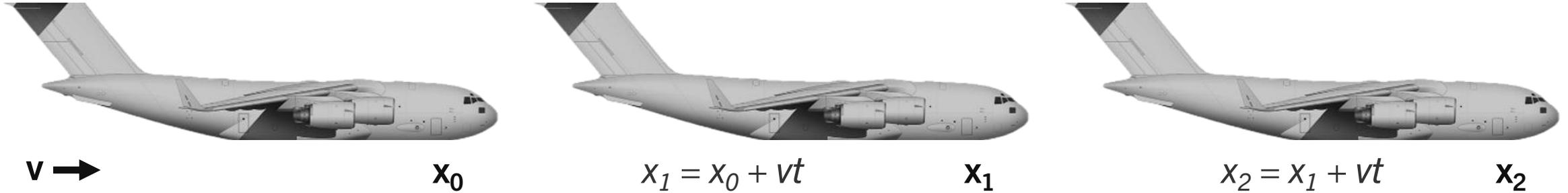
Plane moving at constant velocity

Cycles indicate behavioral patterns



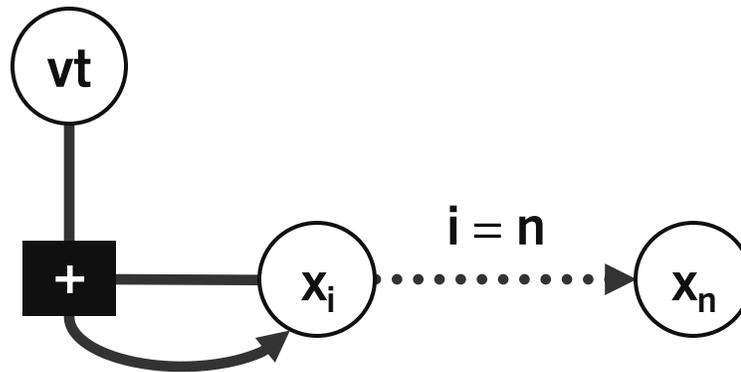
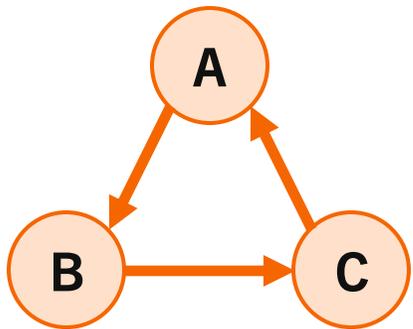
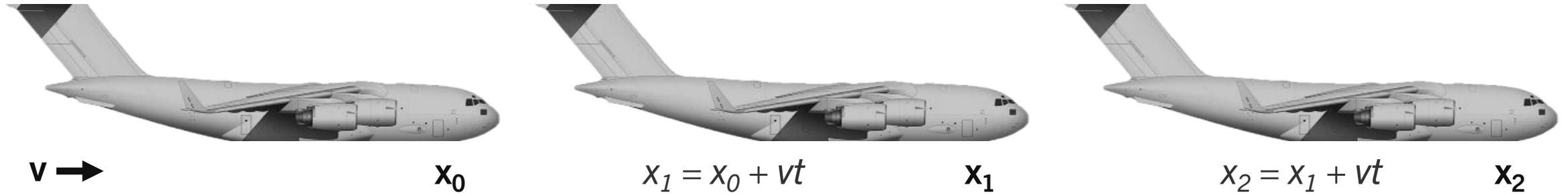
x_0 , x_1 , and x_2 are all different nodes

Cycles indicate behavioral patterns



A more expressive way to show this is $x_{i+1} = x_i + vt$ (unraveling)

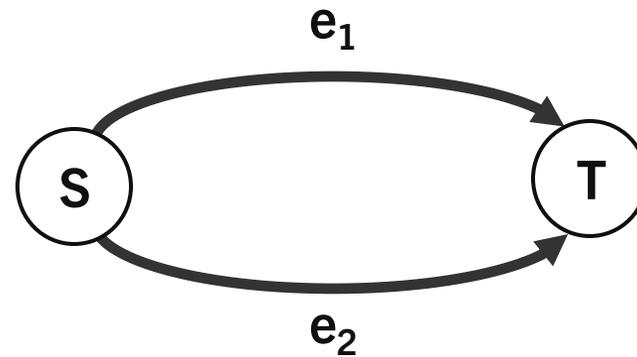
Unraveling requires an exit condition to be solvable



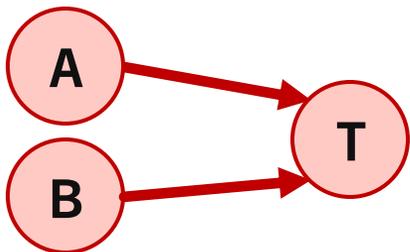
The partial edge shows which edges of x_i are mapped to x_n

Multi-edges indicate competing models

 Ansys

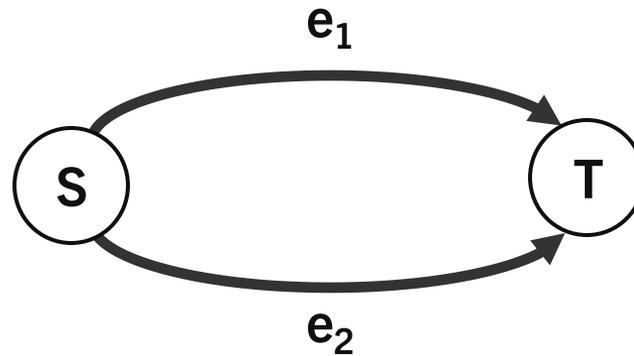


 ChatGPT

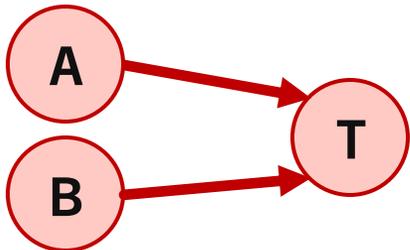


Both edges are viable (“correct”), but only one can be selected for simulation

Ansys



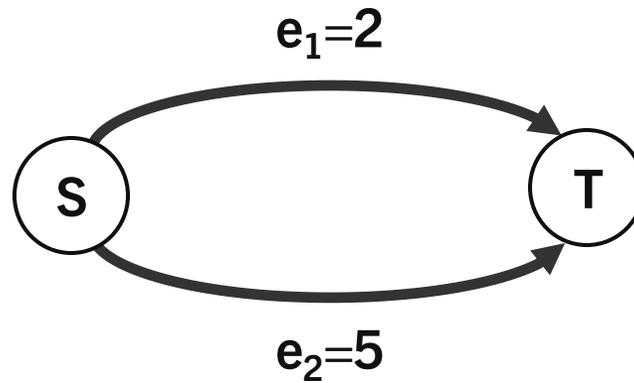
 ChatGPT



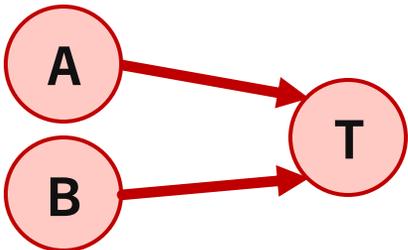
Differences might be on accuracy, computation time, software availability, etc.

Weights allow the agent to *prefer* one edge to another

Ansys



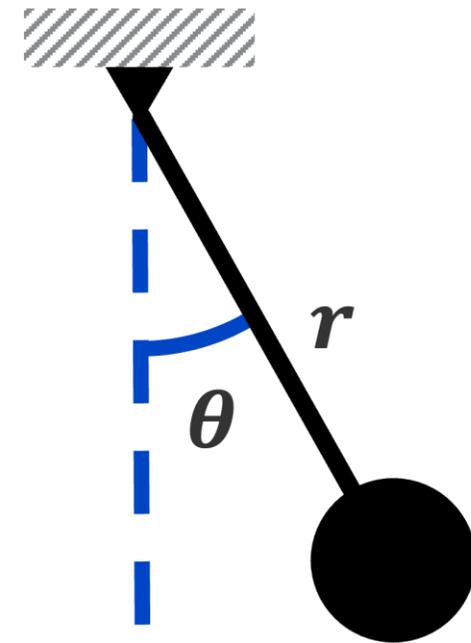
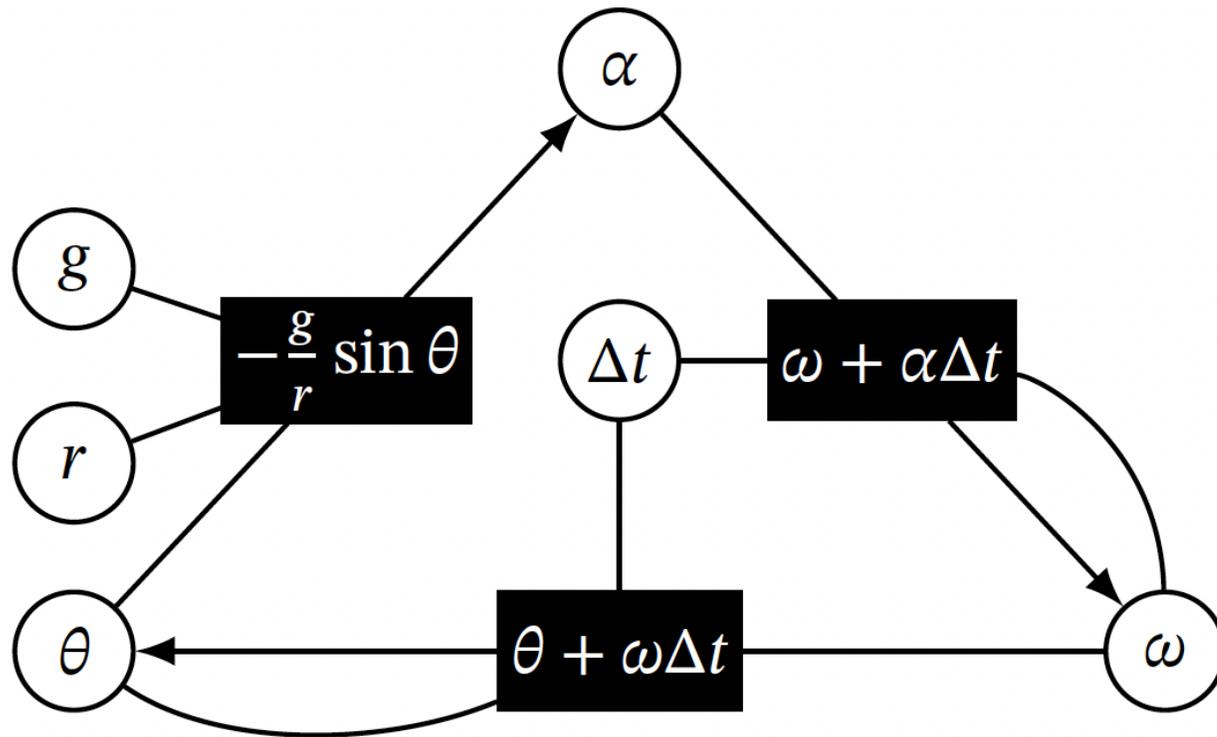
ChatGPT



Demonstration

Universal System Simulation via Constraint Hypergraphs

Pendulum System



Declarative simulation provided by ConstraintHg



constrainthg 0.2.4

```
pip install constrainthg
```

Kernel for building and simulating constraint hypergraphs.

Navigation

Project description

Release history

Download files

Project description



DOI 10.5281/zenodo.17251382 docs passing tests 31/31 release v0.2.4 last commit last tuesday



Search

SOFTWARE

Quickstart

Tutorial

API

Node

Edge

Hypergraph

Relations Module

About

Demos

Repository

CONSTRAINT HYPERGRAPHS

CHG Overview

Learn About CHGs

Quickstart

Use [PIP](#) to install ConstraintHg into your Python environment:

```
pip install constrainthg
```

From there you'll want to import the library into your Python script. This is a pretty typical method to use:

```
from constrainthg.hypergraph import Node, Hypergraph
import constrainthg.relations as R
```

Simple Demo

Note that this demo is found in [demos/demo_basic.py](#)

Let's build a basic constraint hypergraph of the following equations:

- $A + B = C$
- $A = -D$
- $B = -E$
- $D + E = F$
- $F = -C$



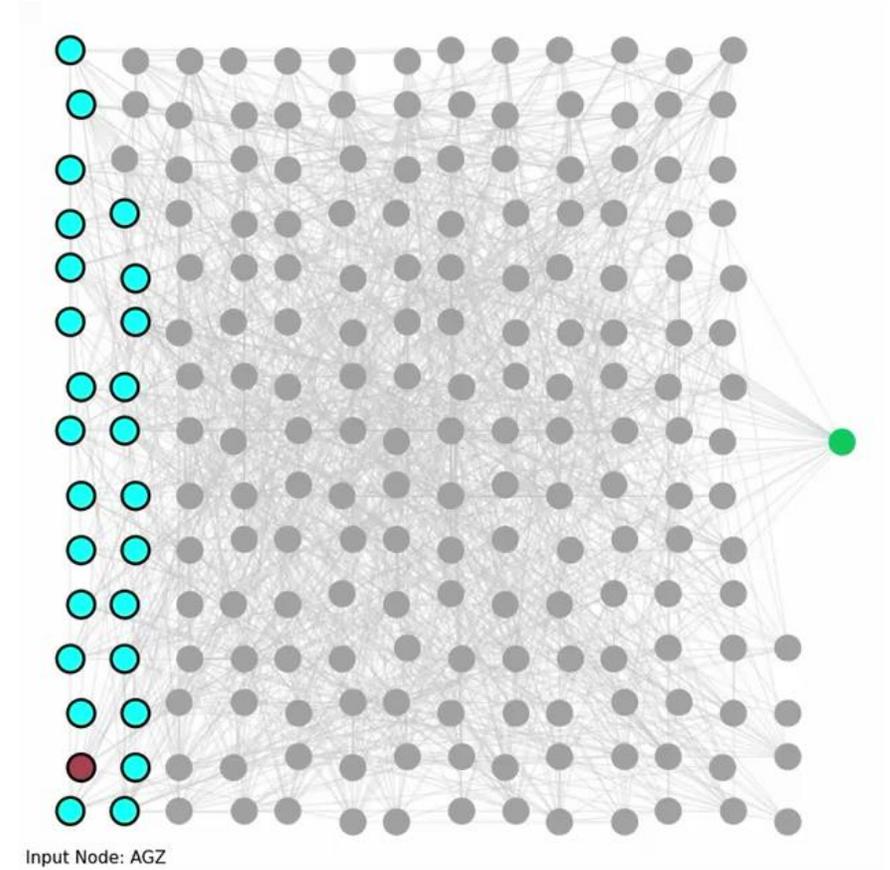
latest



ConstraintHg Functionality

Provides methods for:

- Representing and visualizing CHGs
- Forming cycles, partial edges, and edge weights
- Pathfinding for declarative simulation
 - Extensive logging tools
- Merging CHGs



Process of making a CHG

1. Identify system facts (nodes)

Parameters, application variables, API tokens, etc.



2. Form relations (edges) between nodes

Relations show how one node is determined by a set of other nodes



3. Pass to CHG solver

Solver parses the CHG



4. Request simulation

Solver simulates requested output by finding the shortest path mapping it to a set a known inputs



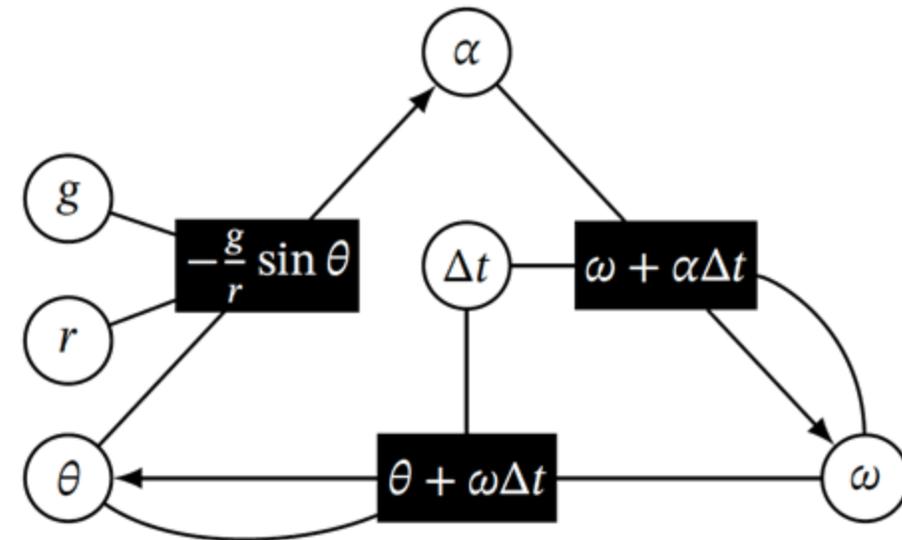
Declarative simulation requires only start & end points

```
hg.solve(  
  target='theta',  
  inputs=(  
    theta=0.785,  
    omega=0.0,  
    g=9.81,  
    r=0.25,  
    delta_t=0.02  
  ),  
  min_index=2,  
)
```

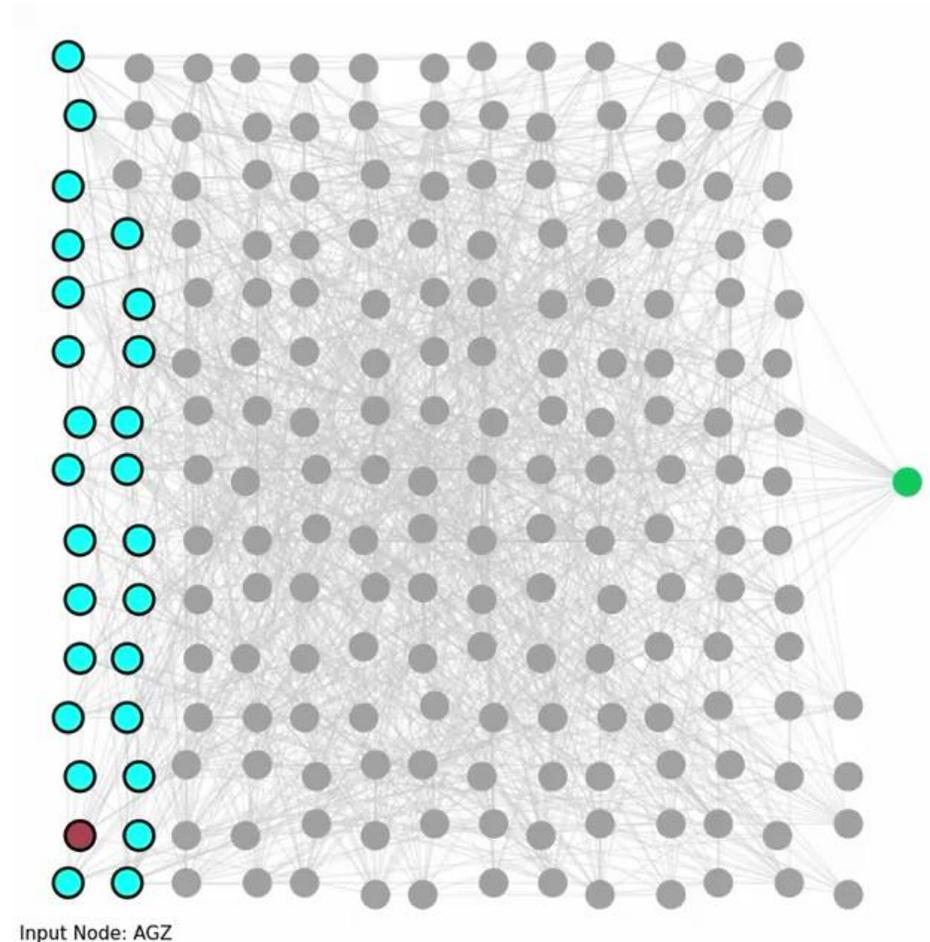
Simulation call

```
└─theta(2)=0.7739  
  └─omega(2)=-0.5547  
    └─alpha(2)=-27.74  
      └─g=9.81  
        └─theta=0.785  
          └─r=0.25  
            └─delta_t=0.02  
              └─omega=0  
                └─delta_t=0.02  
                  └─theta=0.785
```

Discovered, unraveled simulation



Limitation: slow searchability (cannot be presolved)

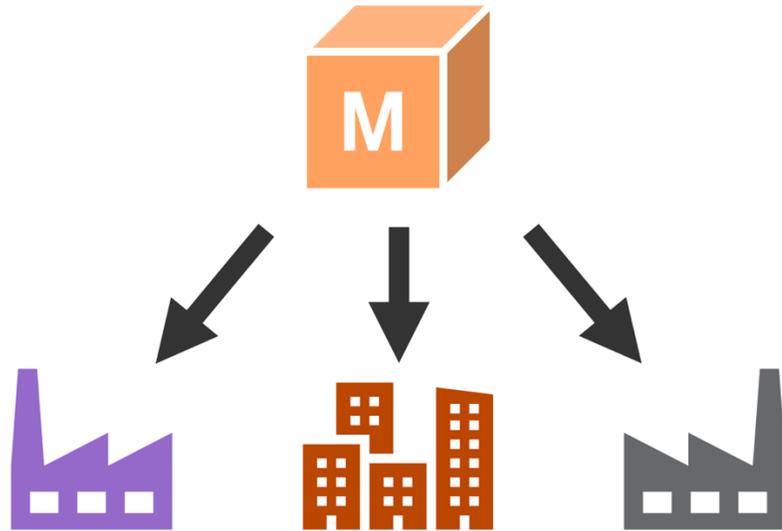


Applications of CHGs

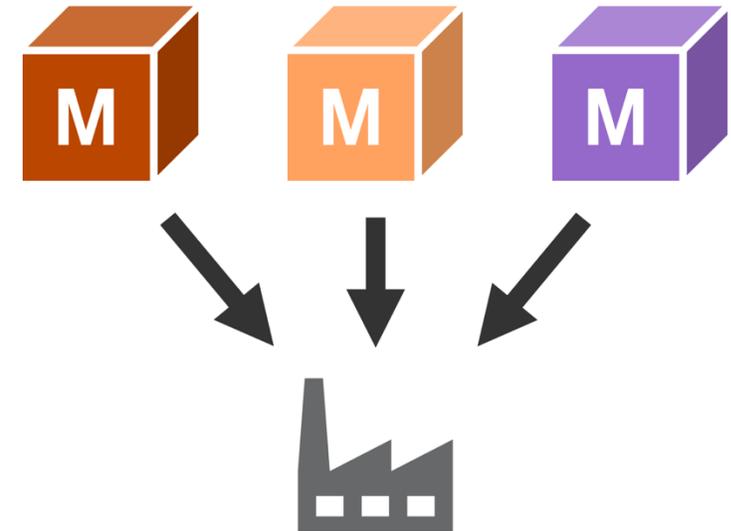
Universal System Simulation via Constraint Hypergraphs

CHGs provide platforms for model-based engineering and digital twins

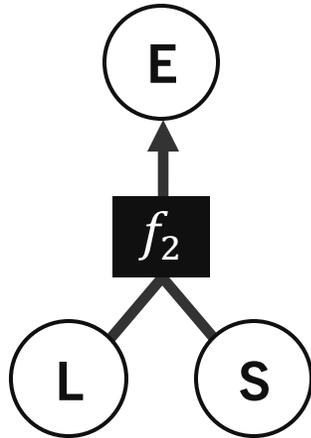
Maintains information in different contexts



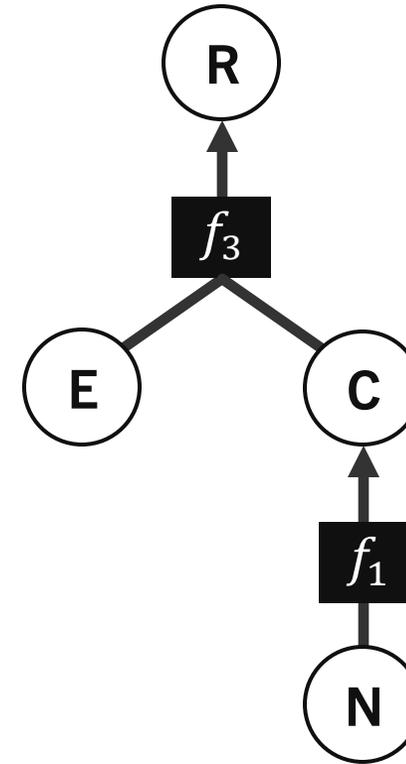
Maintains information with different models



New behaviors can be expressed as new paths in the union of two CHGs

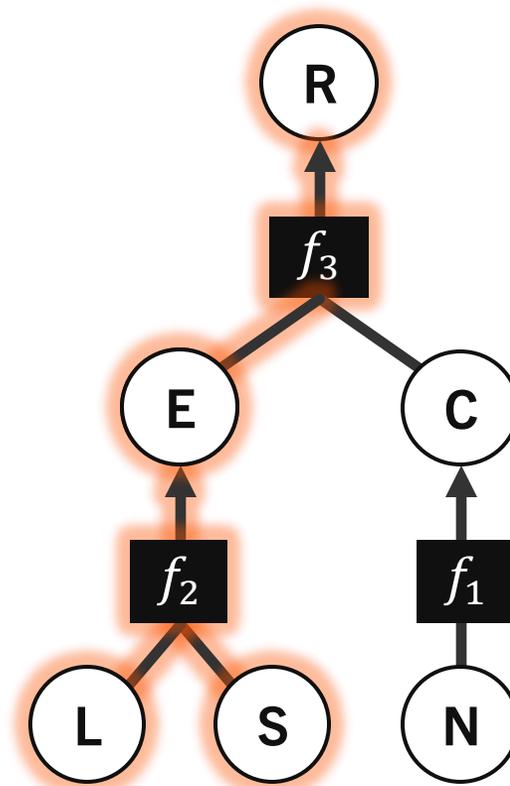


Graph 1



Graph 2

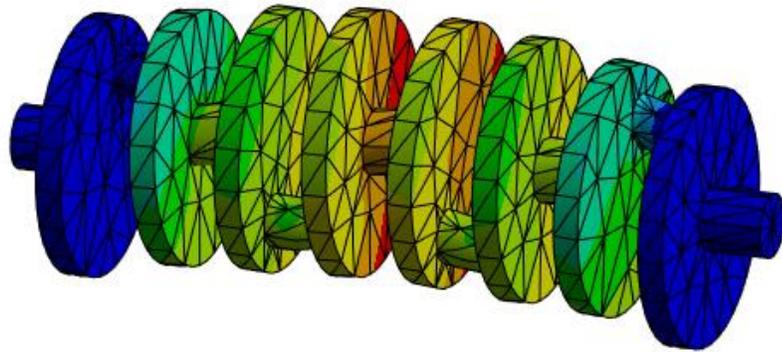
New behaviors can be expressed as new paths in the union of two CHGs



Graph 1 \cup 2

New behaviors include simulation paths that go across calculating software

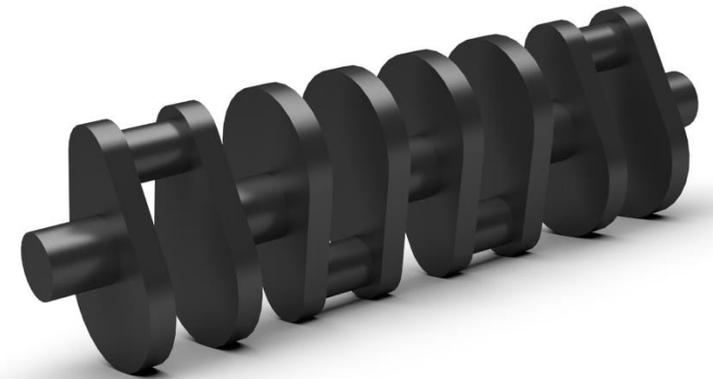
Material Mechanics



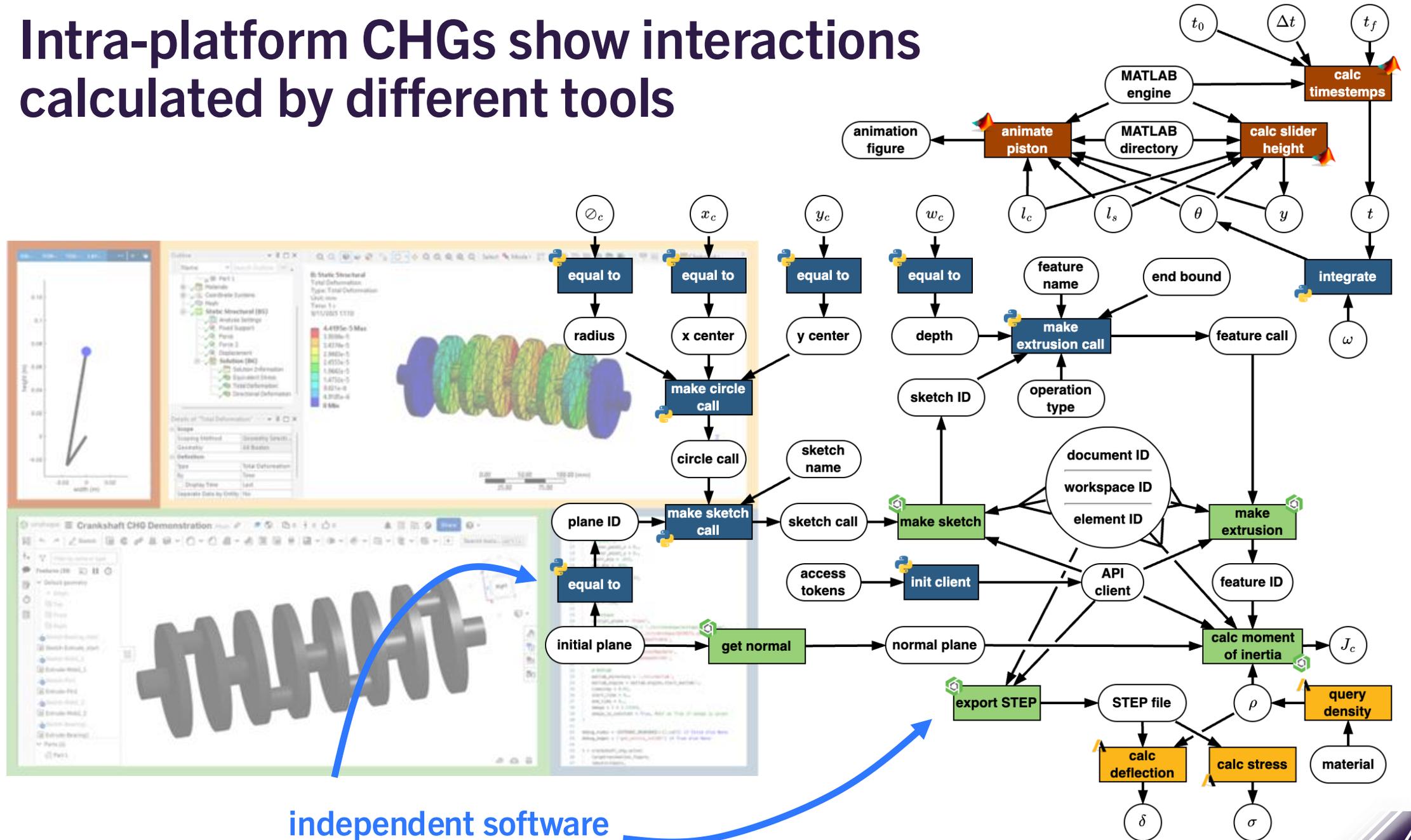
Kinematic Analysis



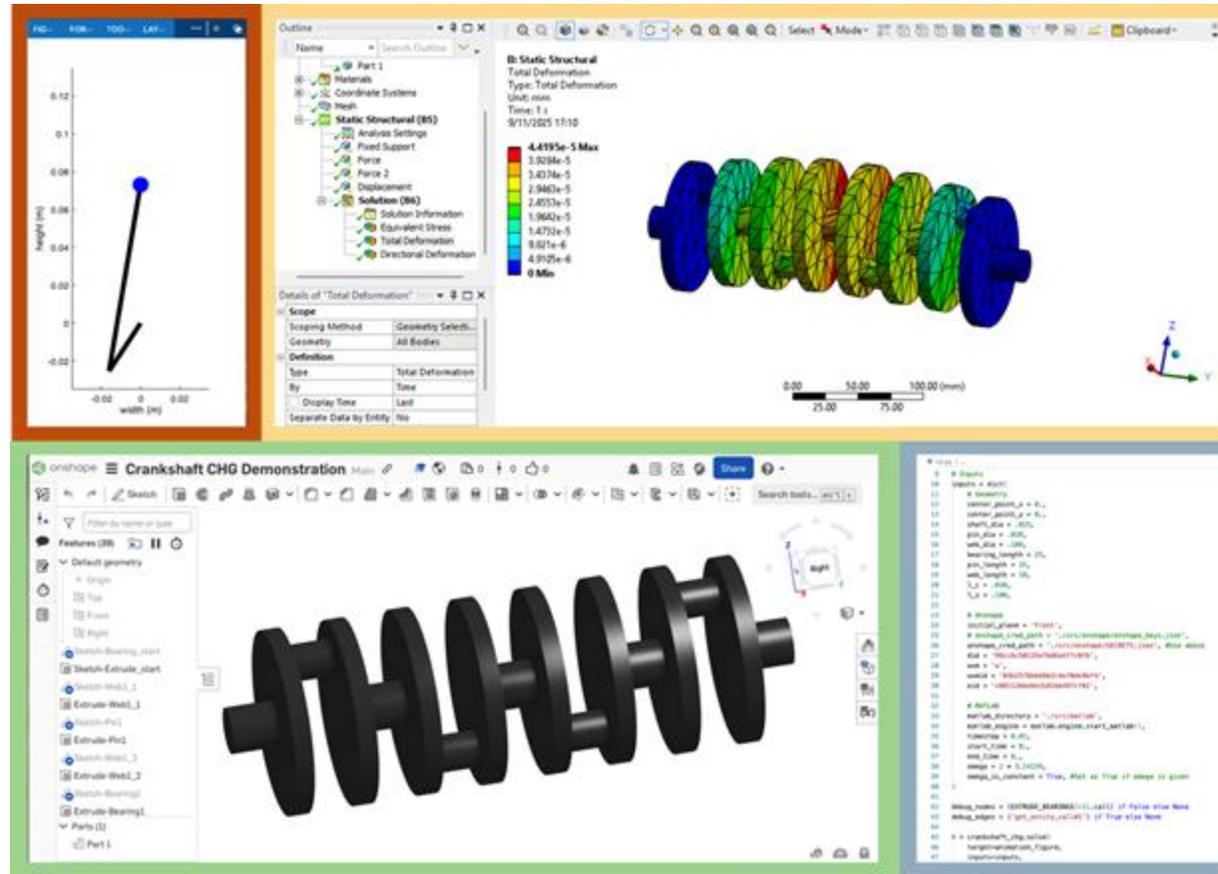
Mass Properties



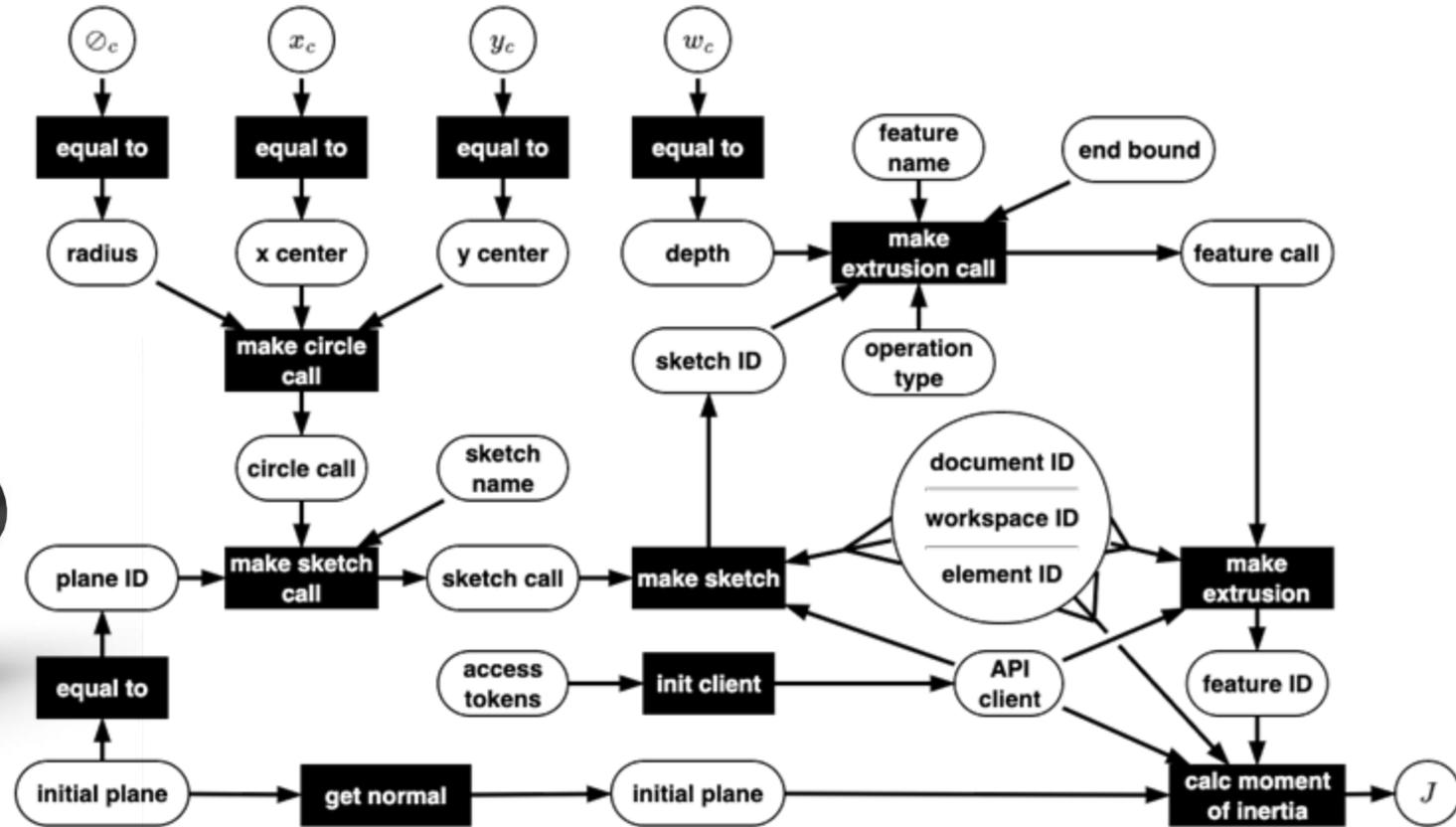
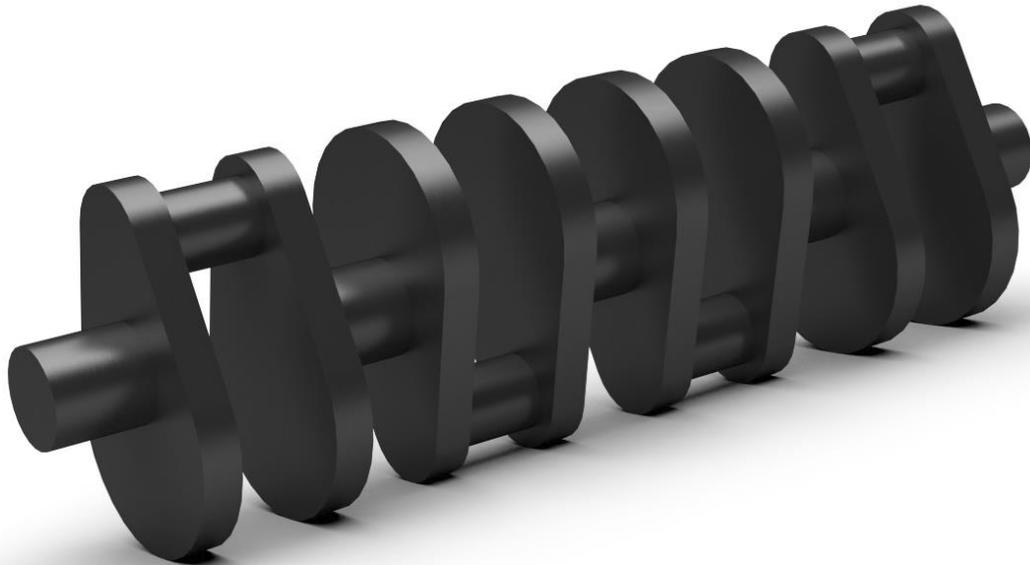
Intra-platform CHGs show interactions calculated by different tools



Representing software calculations as edges makes executable digital threads simpler



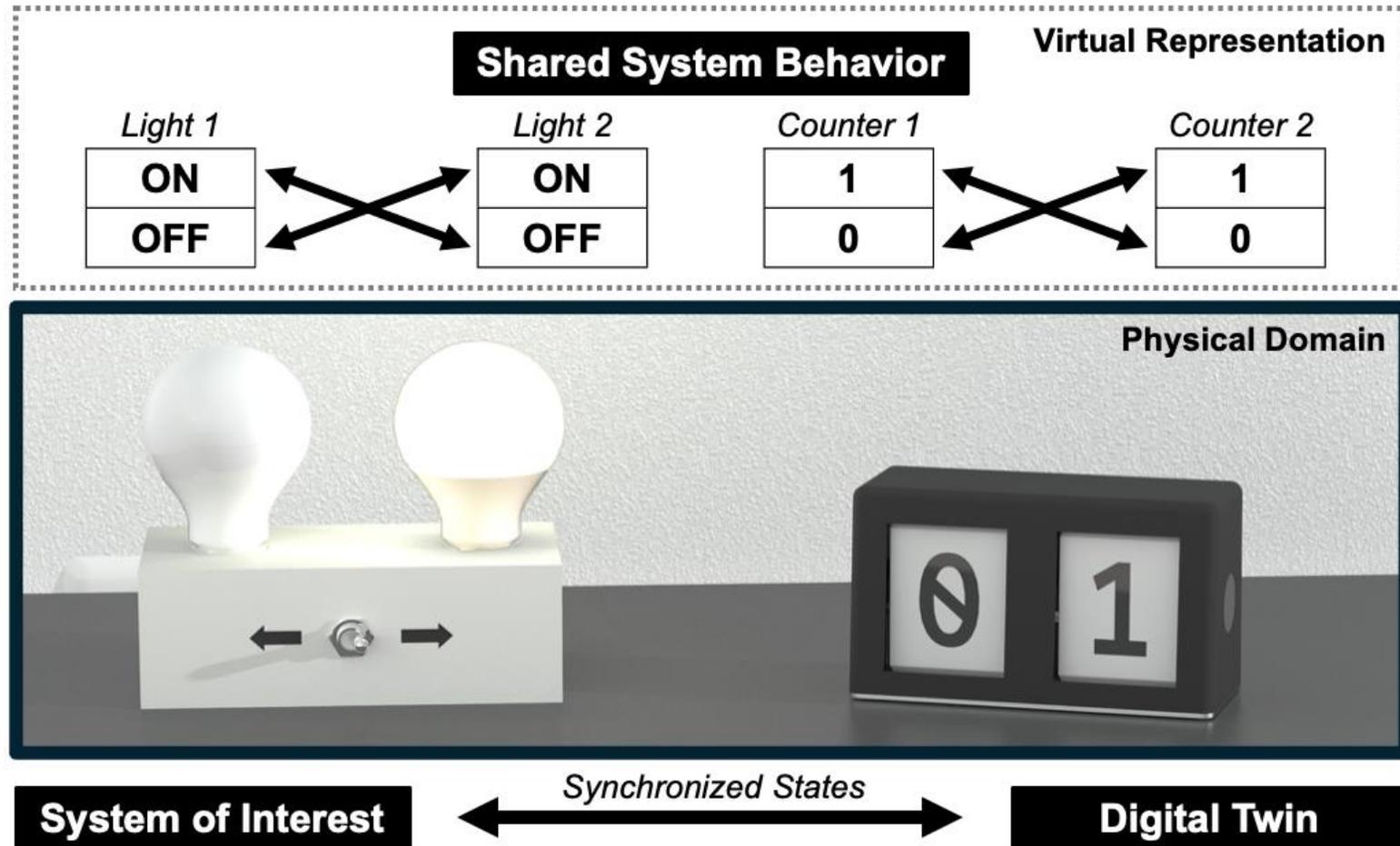
Limitation: not focused on being human readable



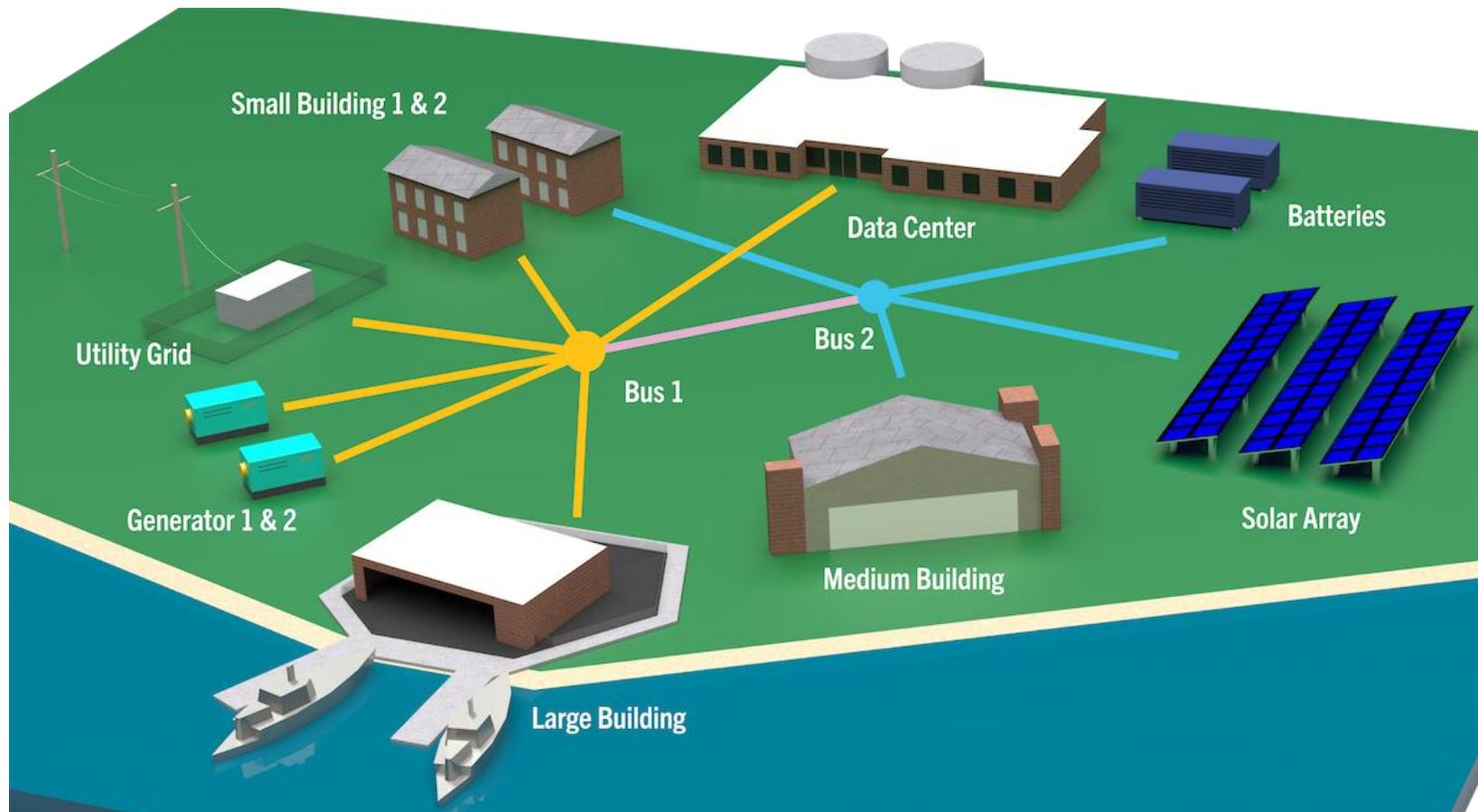
DTs are systems synchronized with another system of interest



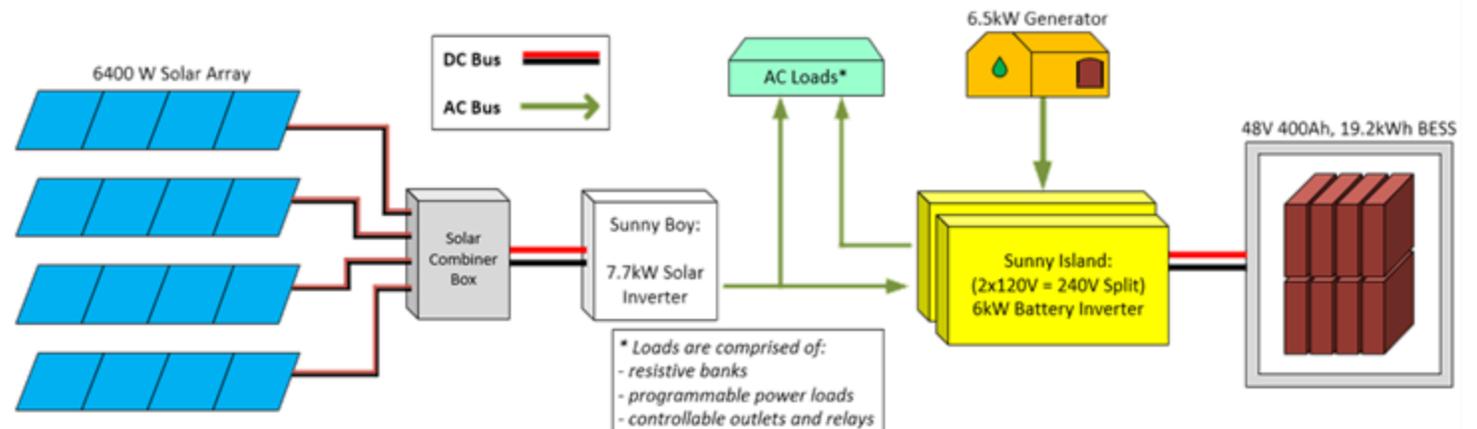
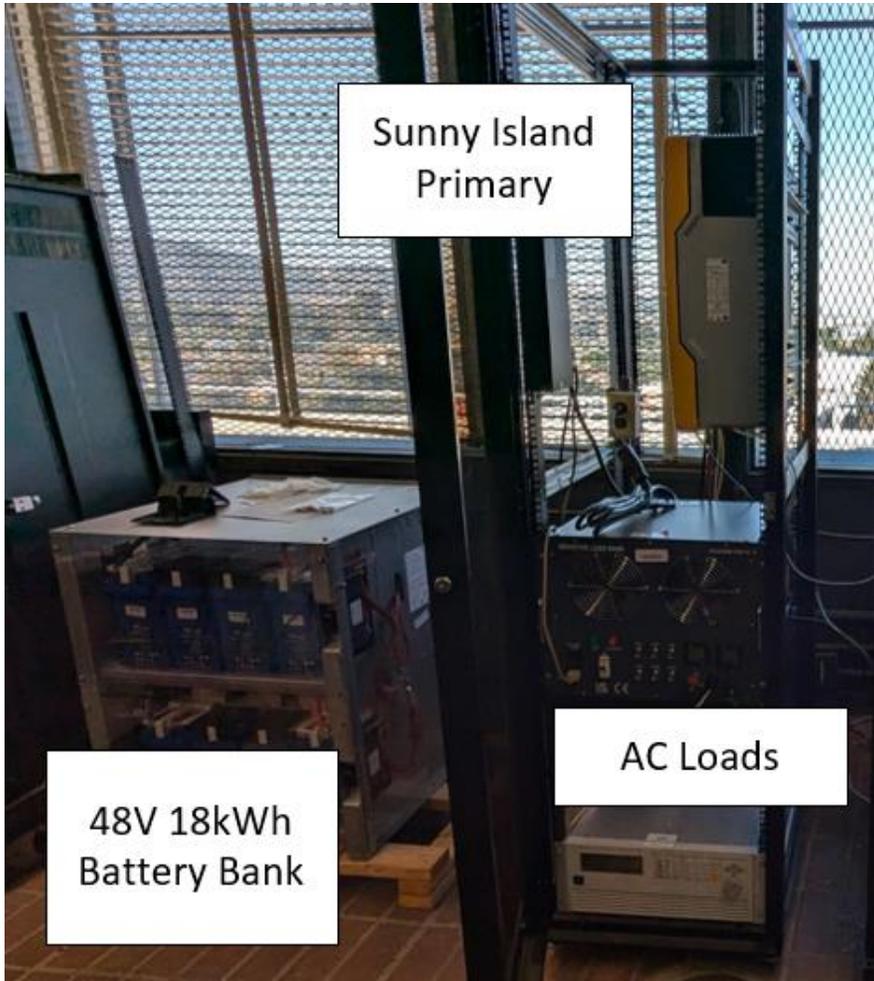
Digital Twins are 2 systems sharing the same CHG



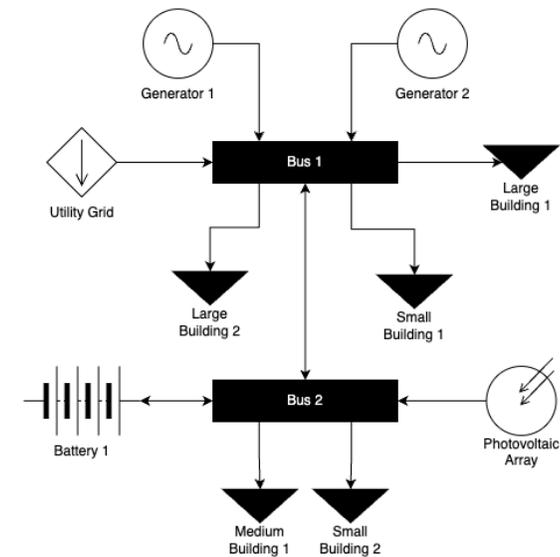
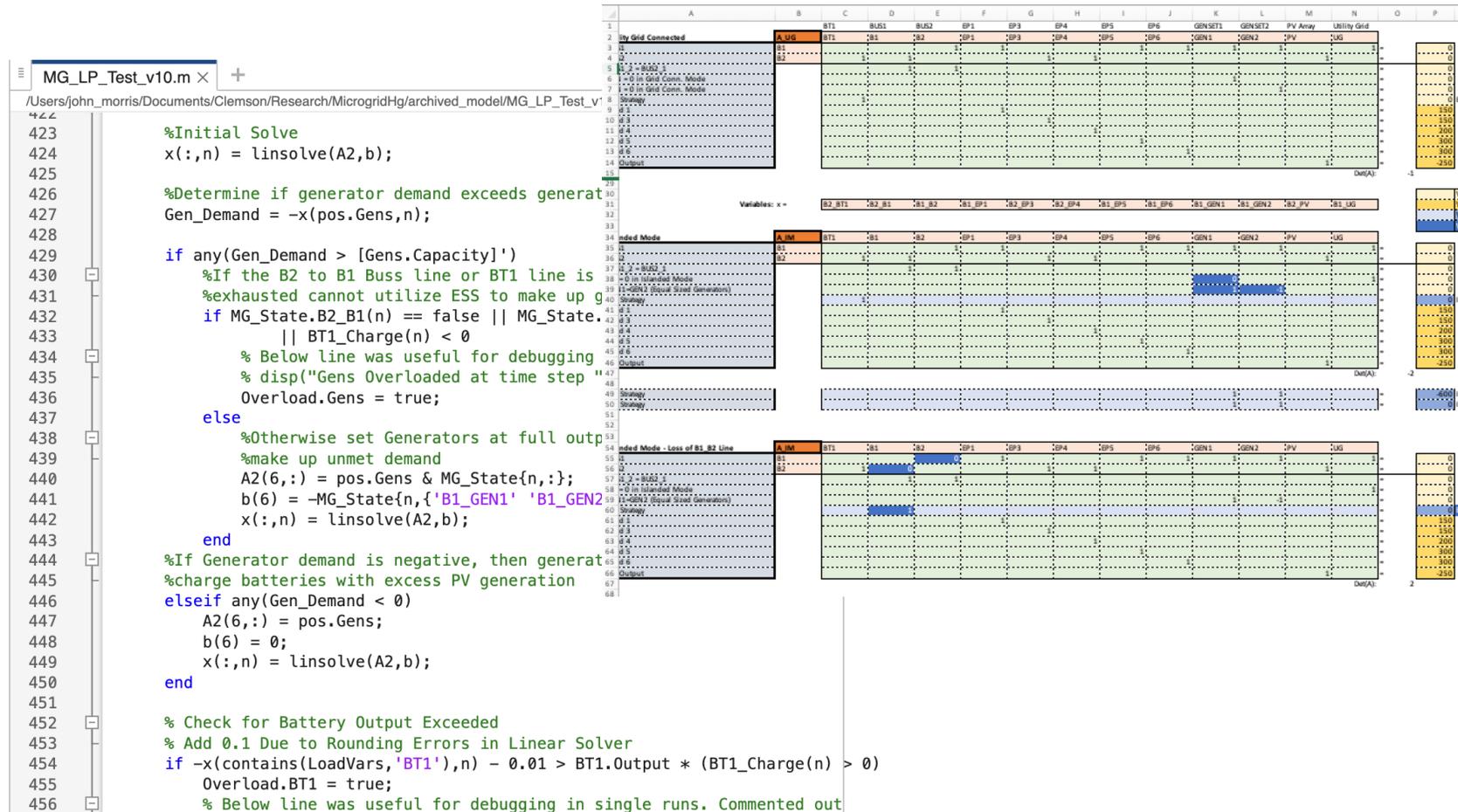
Demonstration: Naval Microgrid Digital Twin



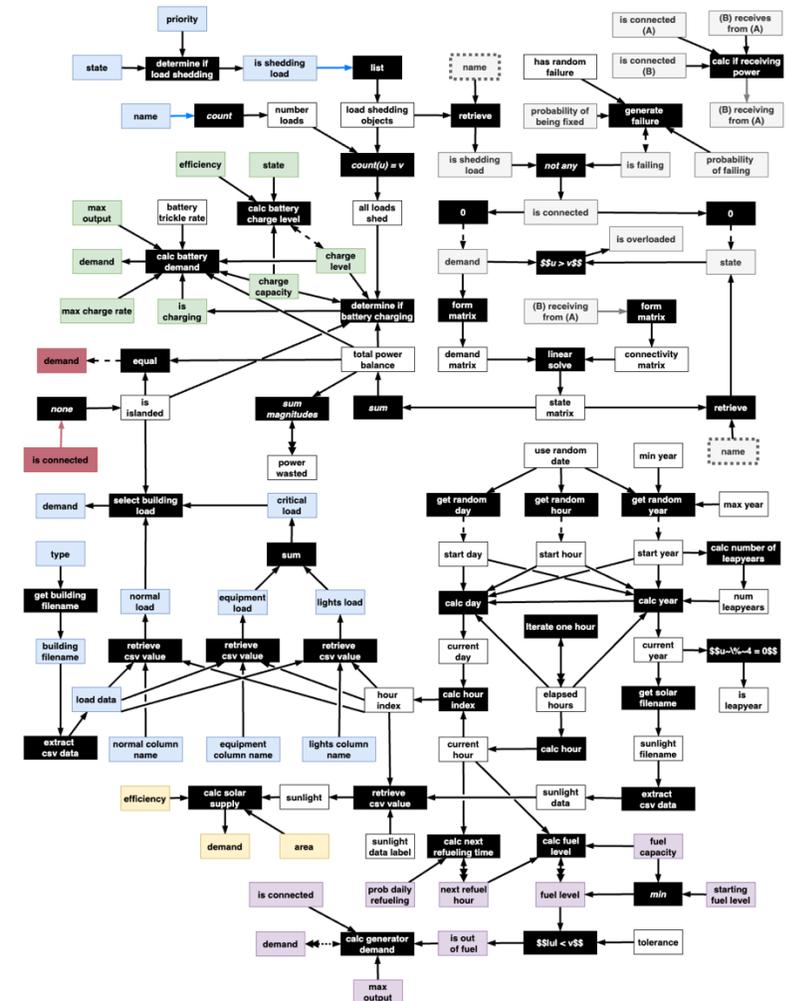
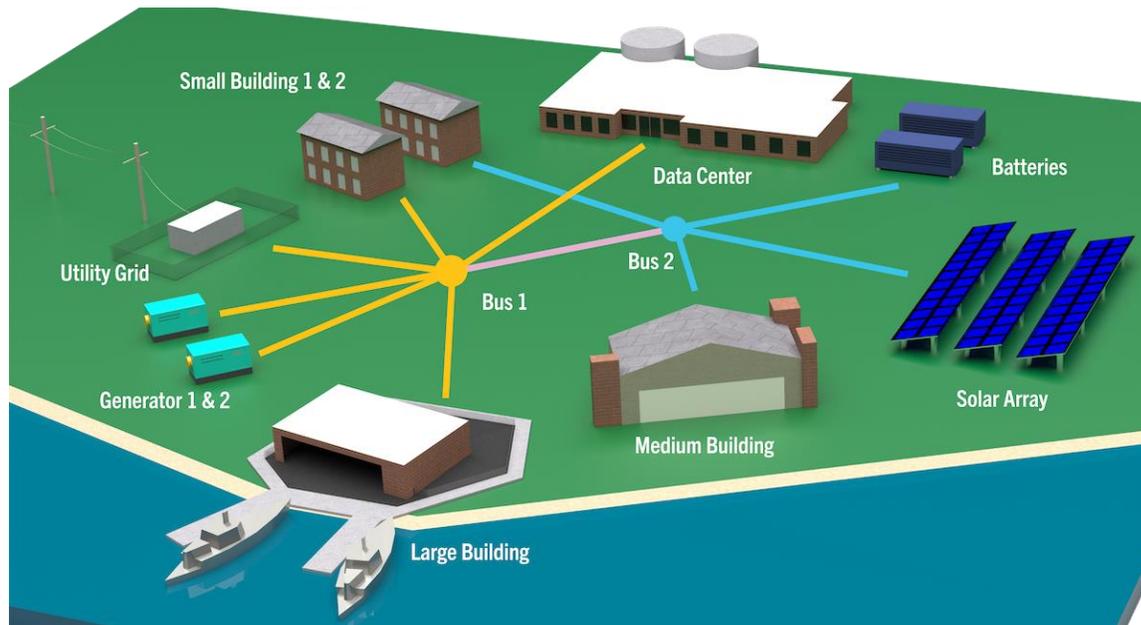
Physical Microgrid at Naval Postgraduate School



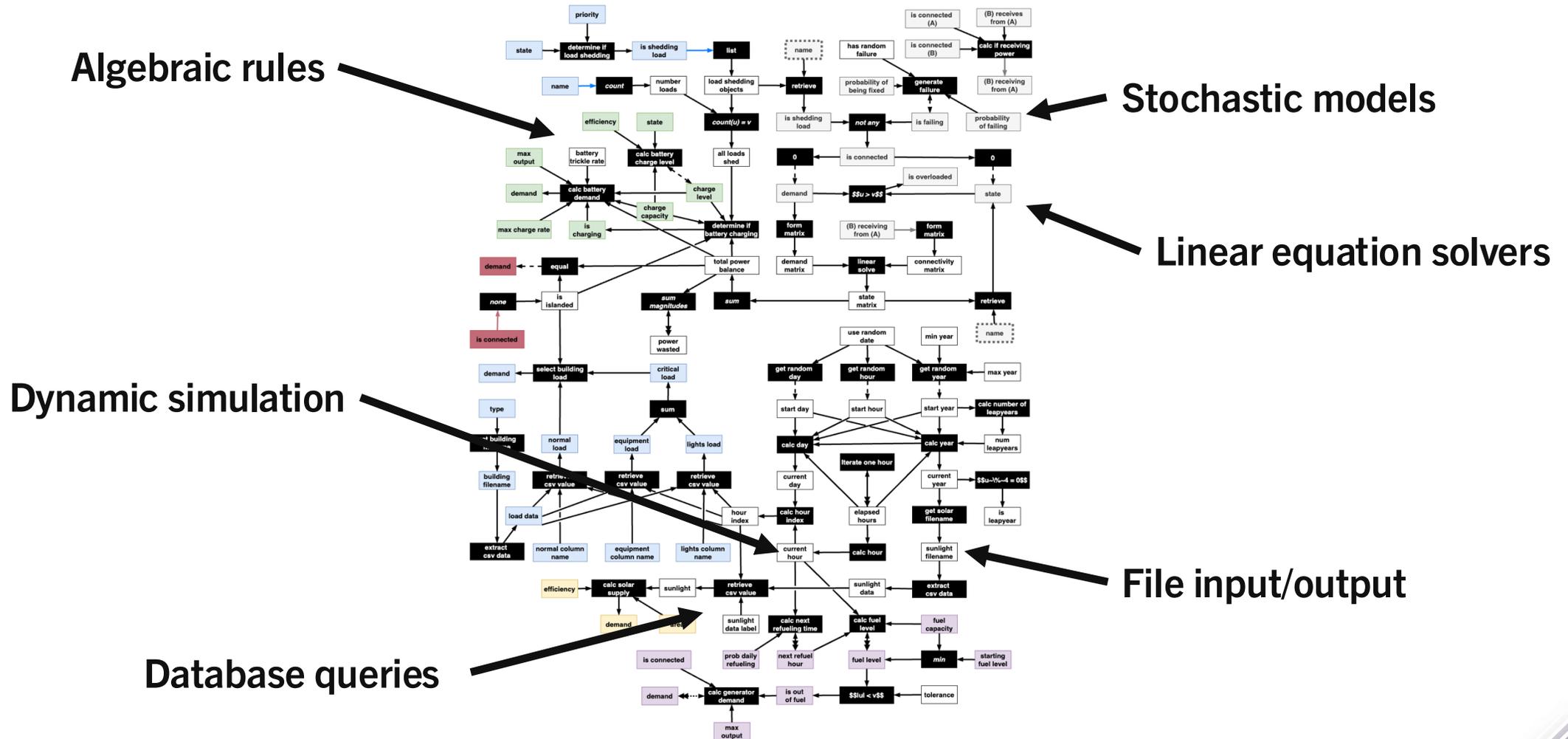
Previous Imperative Modeling of Microgrid



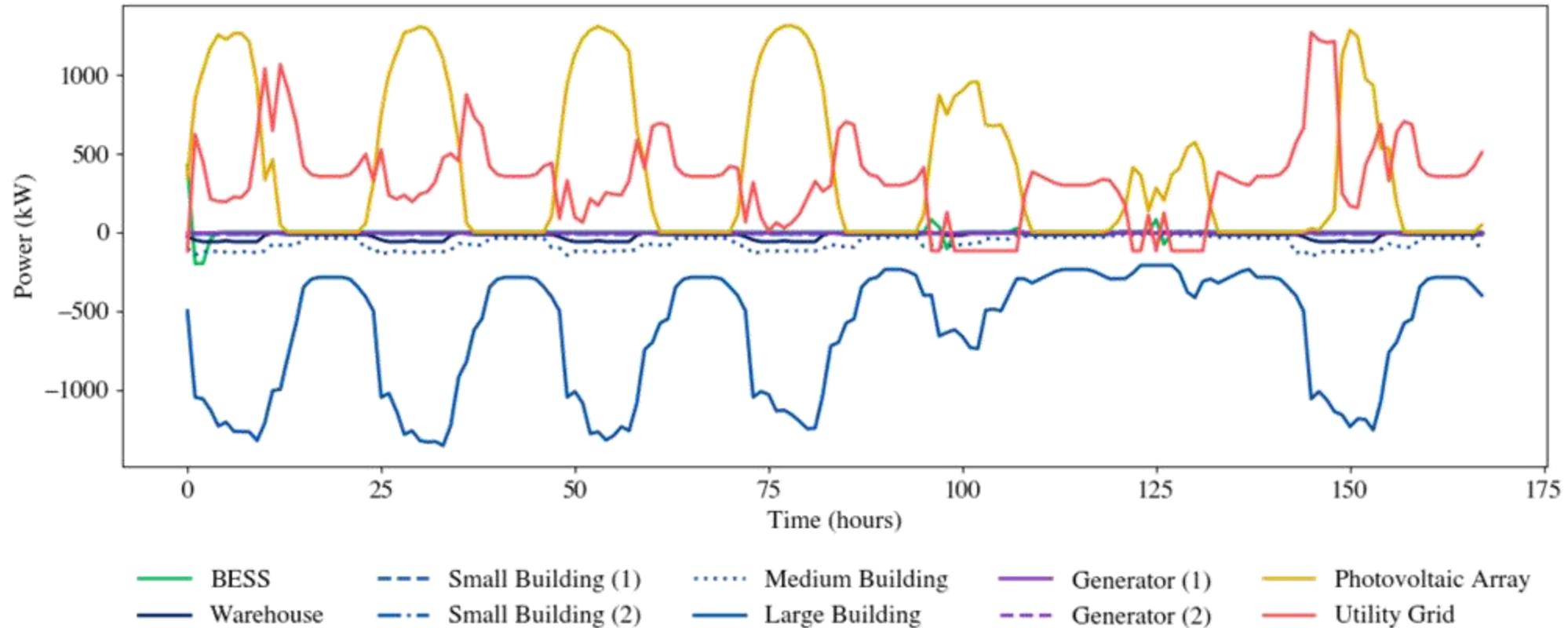
Transformed CHG contains 594 nodes and 334 edges



Includes all kinds of simulation and modeling



Autonomously observes and simulates the real system



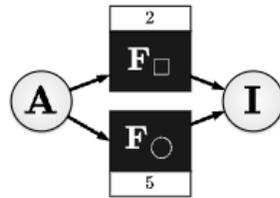
Future work: best practices for model selection

Model Selection

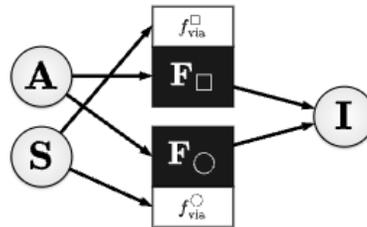
Abstracted Behavior



Model Preferences



Viability statements



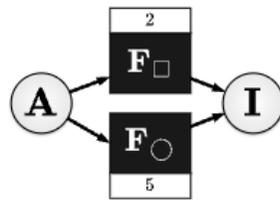
Future work: heuristic search methods

Model Selection

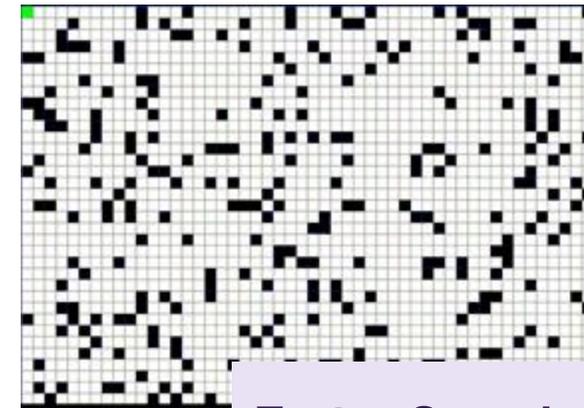
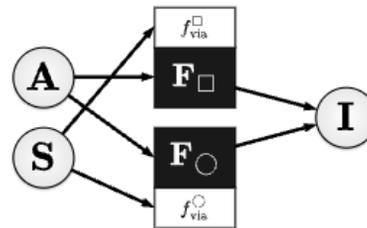
Abstracted Behavior



Model Preferences



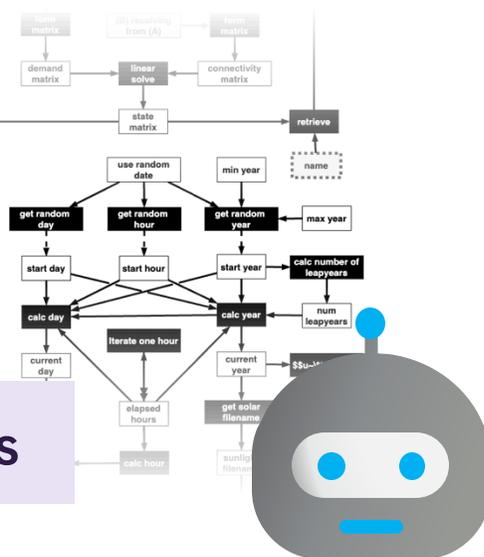
Viability statements



Wgullyn, 2021

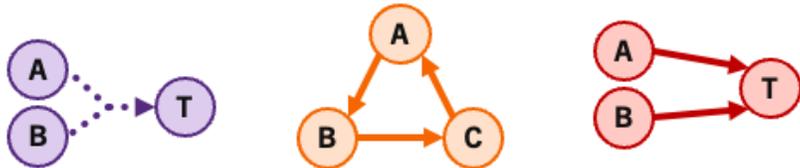
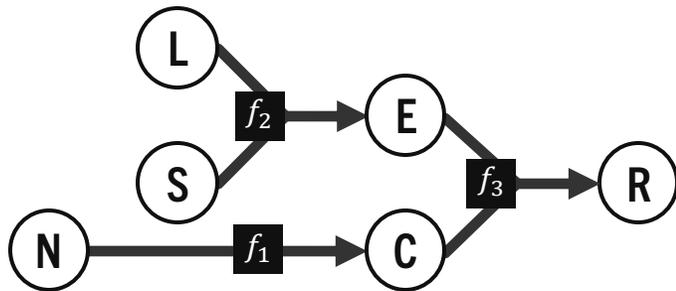
Faster Search Methods

Neural Nets + CHGs



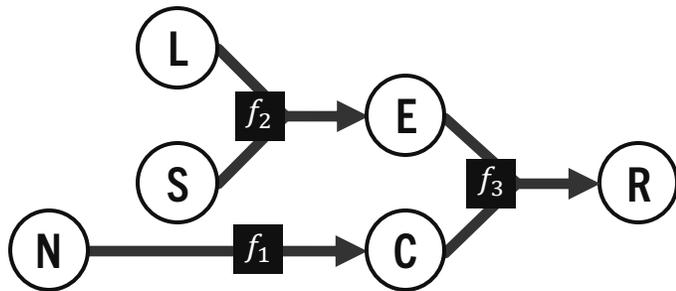
The structure of a CHG allows it to represent any system

Universal Modeling

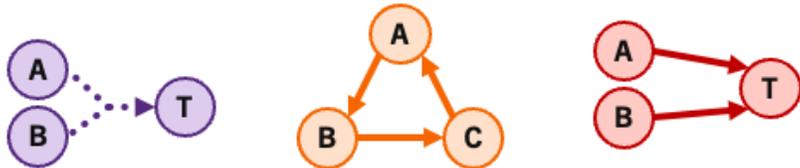


Information about a system can be discovered autonomously

Universal Modeling

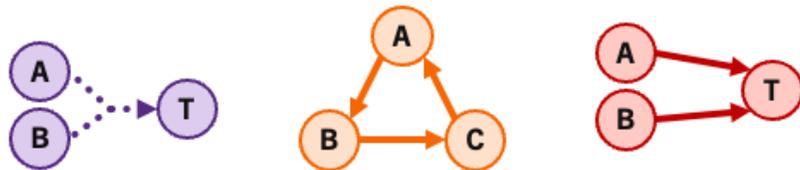
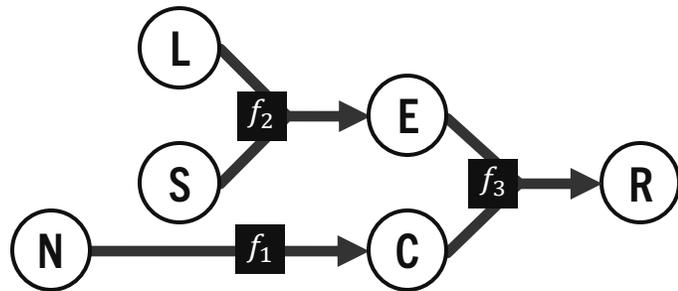


Declarative Simulation



Models can be connected across domains, scales, and even tools

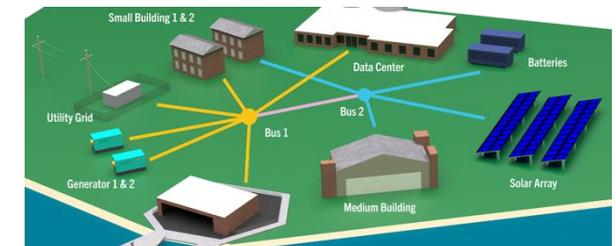
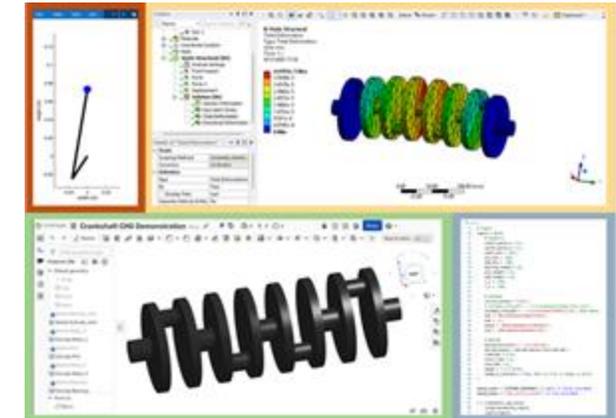
Universal Modeling



Declarative Simulation

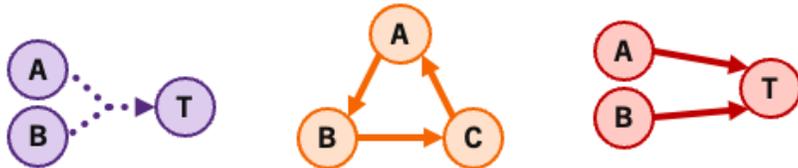
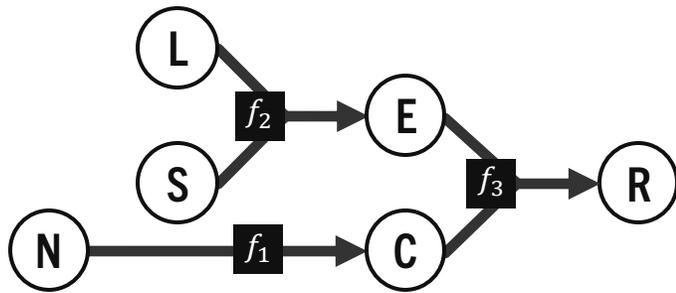


Executable Digital Threads



CHGs provide a universal language for declarative systems modeling

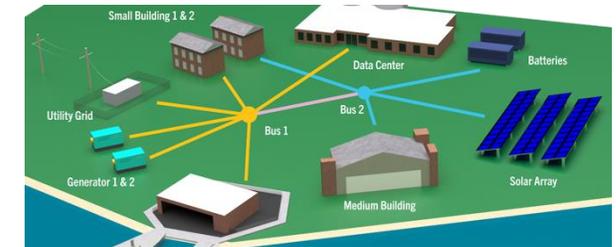
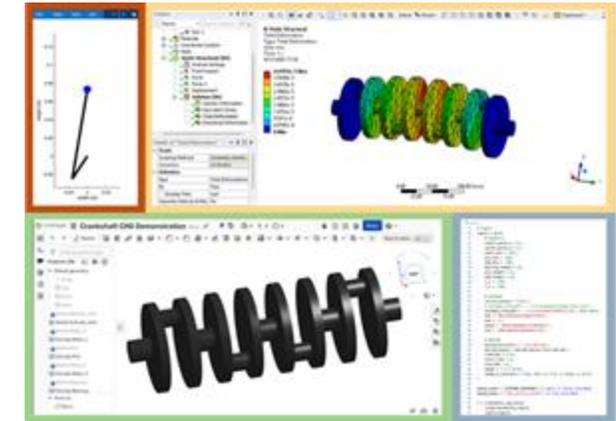
Universal Modeling



Declarative Simulation



Executable Digital Threads

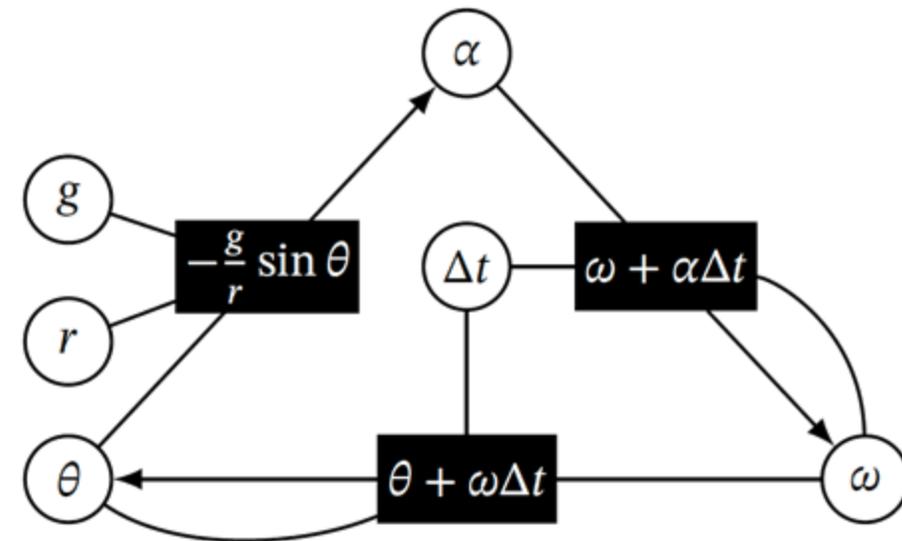


Add Relations

```
def Rtheta_to_alpha(theta, g, r):  
    return -g / r * sin(theta)
```

```
def Rintegrate_omega(omega, alpha, delta_t):  
    return omega + alpha * delta_t
```

```
def Rintegrate_theta(theta, omega, delta_t):  
    return theta + omega * delta_t
```



Add Edges

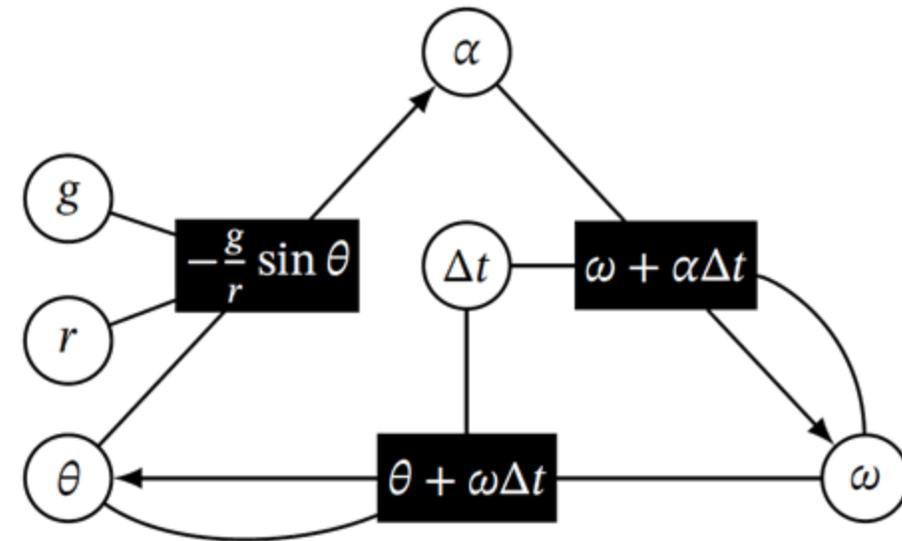
```
hg = Hypergraph()

hg.add_edge(
    sources=('theta', 'g', 'r'),
    target='alpha',
    rel=Rtheta_to_alpha,
)

hg.add_edge(
    sources=('omega', 'alpha', 'delta_t'),
    target='omega',
    rel=Rintegrate_omega,
)

...

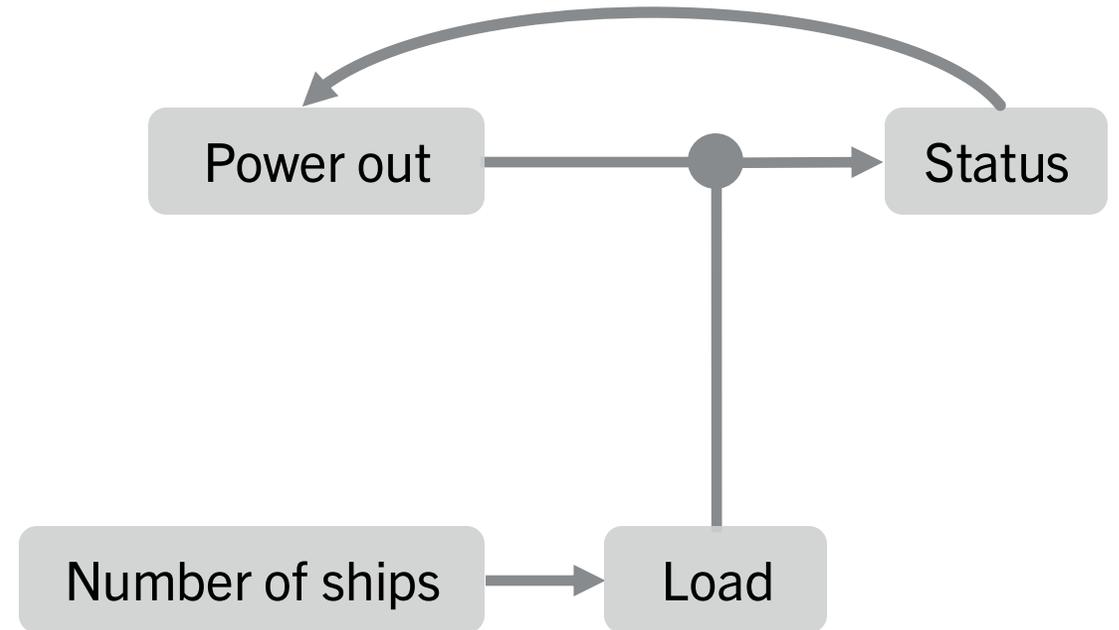
```



Cycles violate transitivity, indicating conflicting models

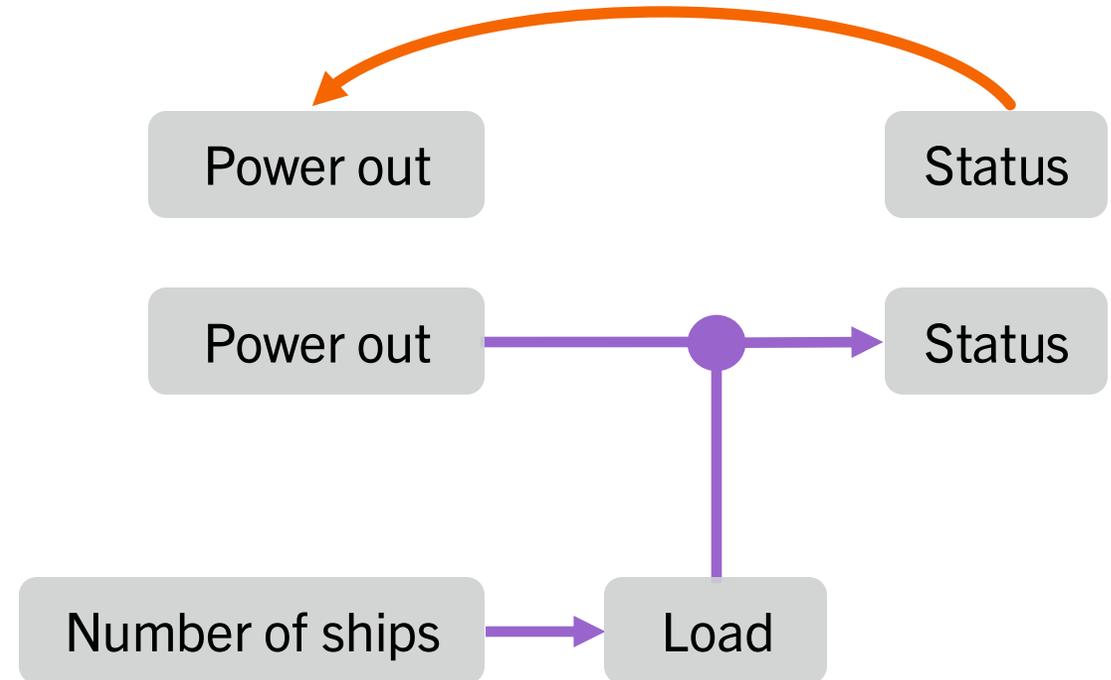
Can be dealt with in two ways:

1. Separation
2. Unraveling



Separating cycles into distinct graphs

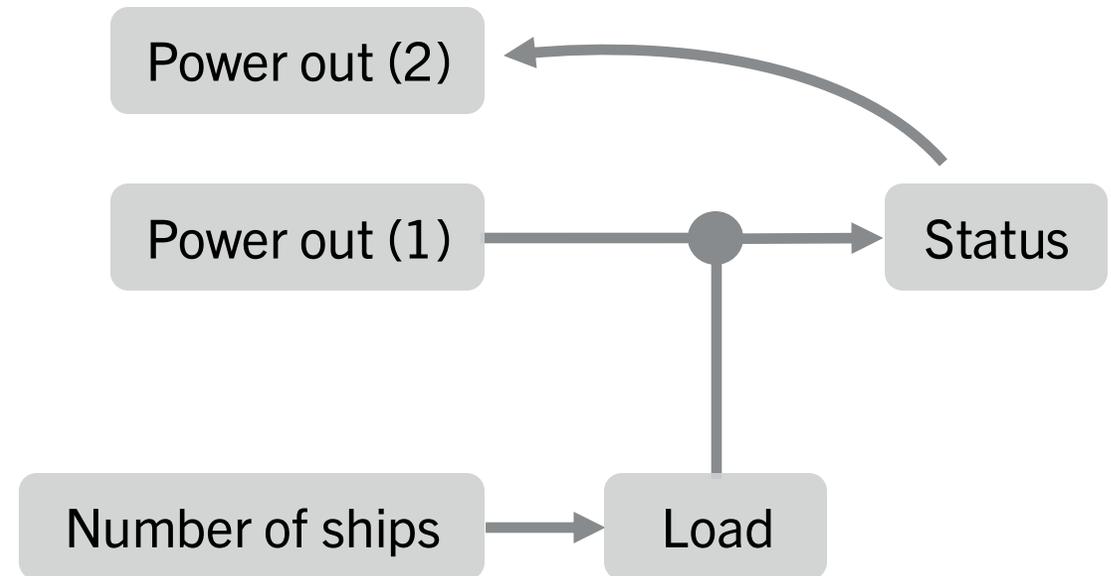
Good for isolating *competing* models



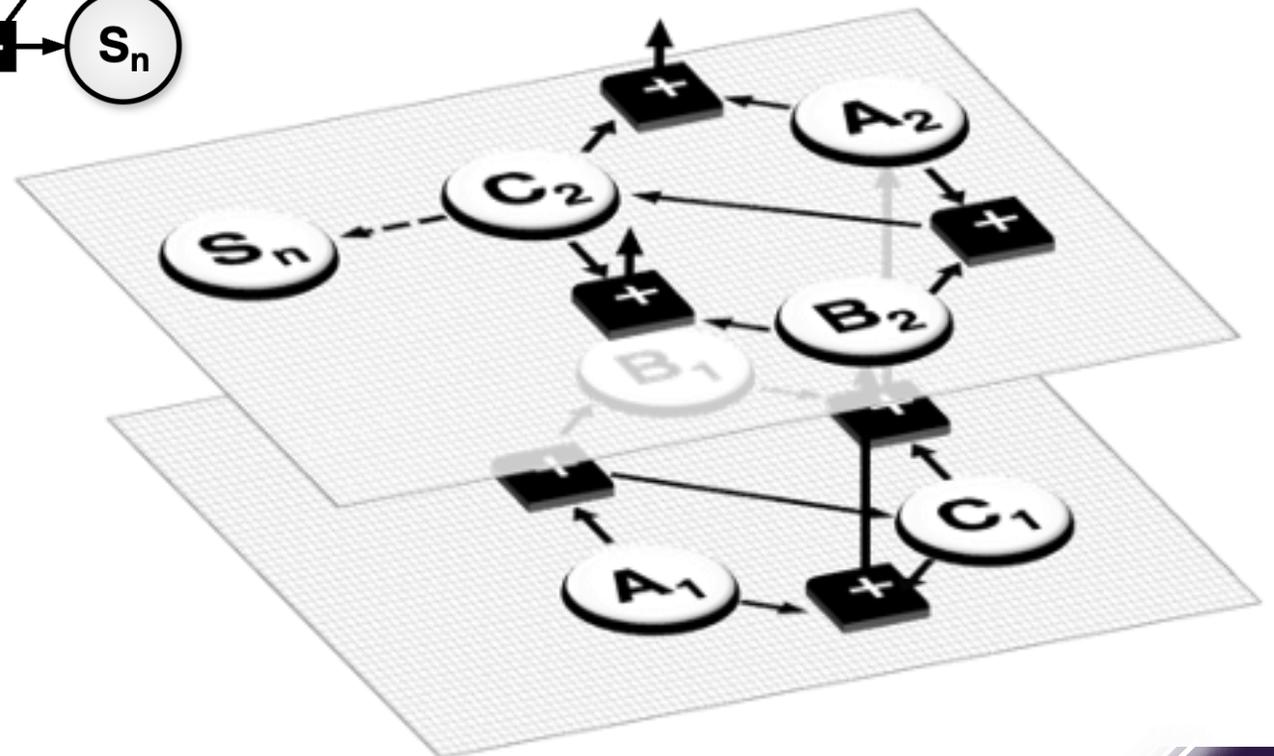
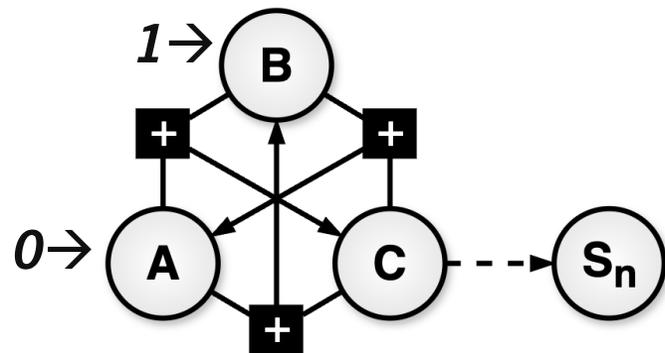
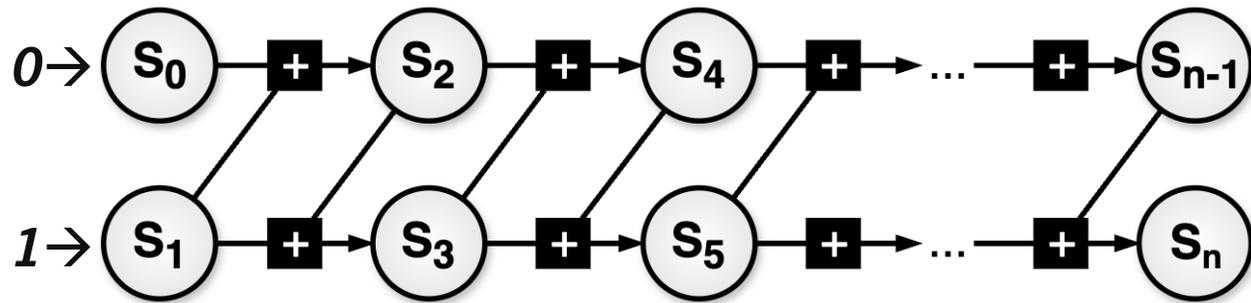
Unraveling nodes allows cycles to extend the hypergraph

Good for *pattern* adaption

Unraveling occurs while searching for simulation paths and requires an exit edge

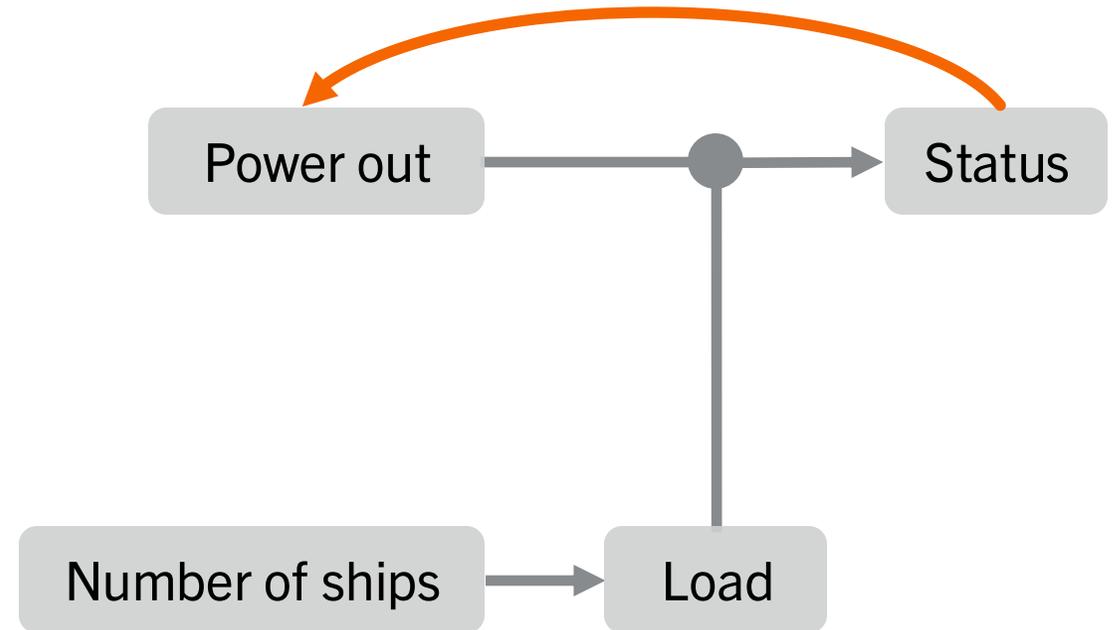


Example computing Fibonacci sequence using cloning



Independent behaviors make the hypergraphs immediately modifiable

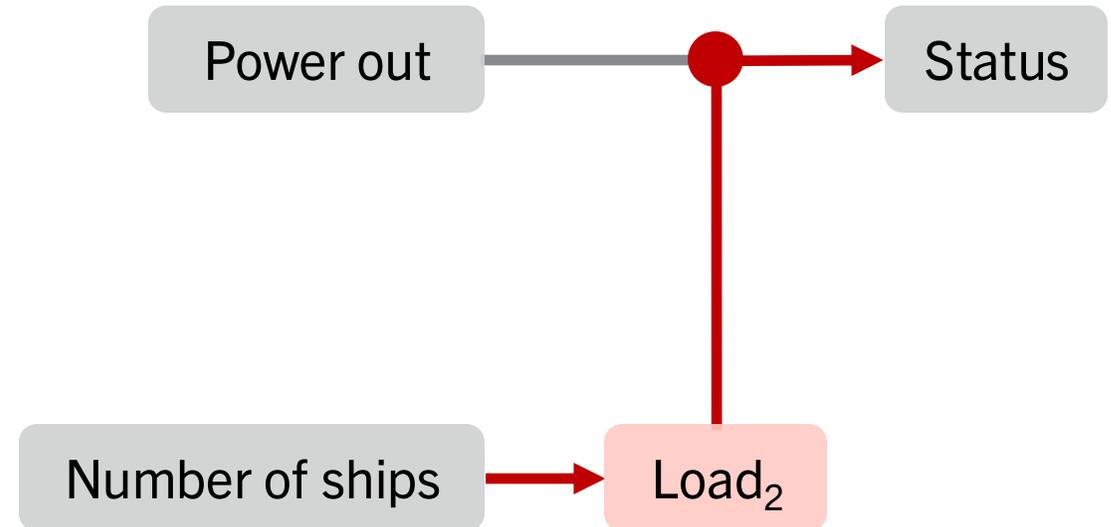
Functions can be rewritten, removed, or added without affecting the consistency of the graph (*no side effects*)



Caveat: scope changes are not guaranteed to be consistent

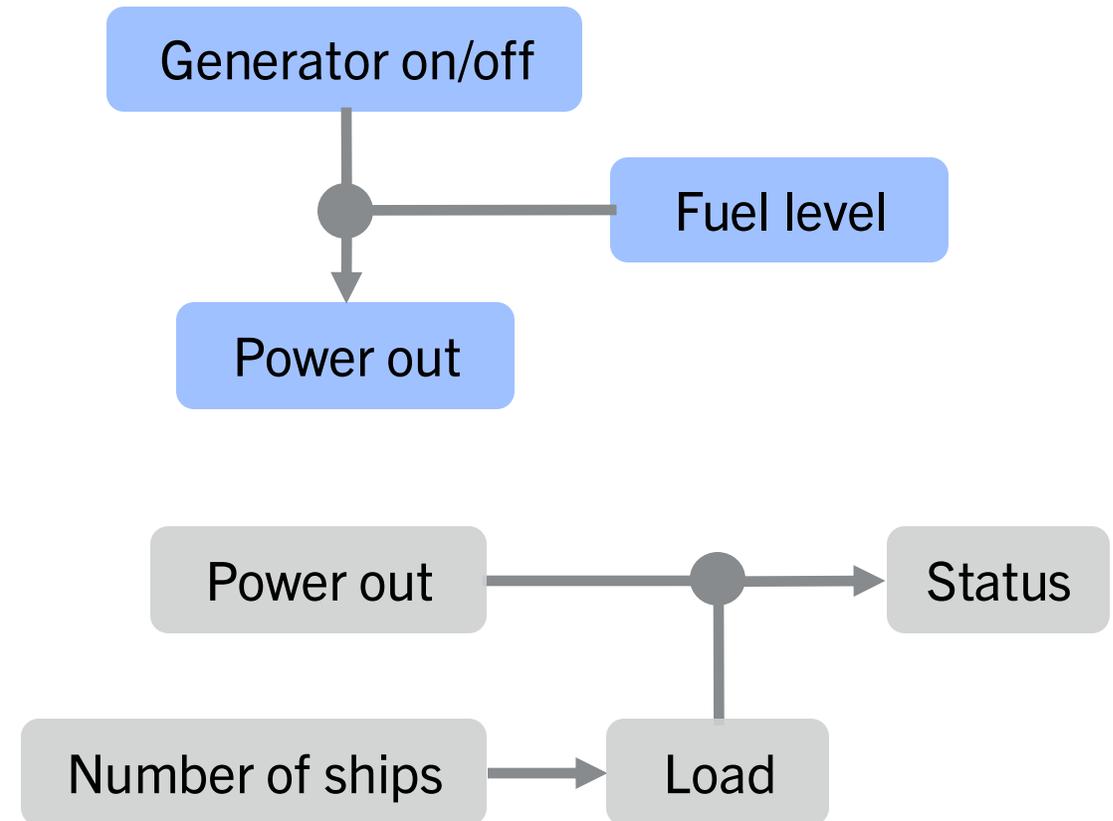
Nodes can be modified only if all connecting edges are also updated to maintain consistency (*only local side effects*)

Behavioral assumptions may be affected



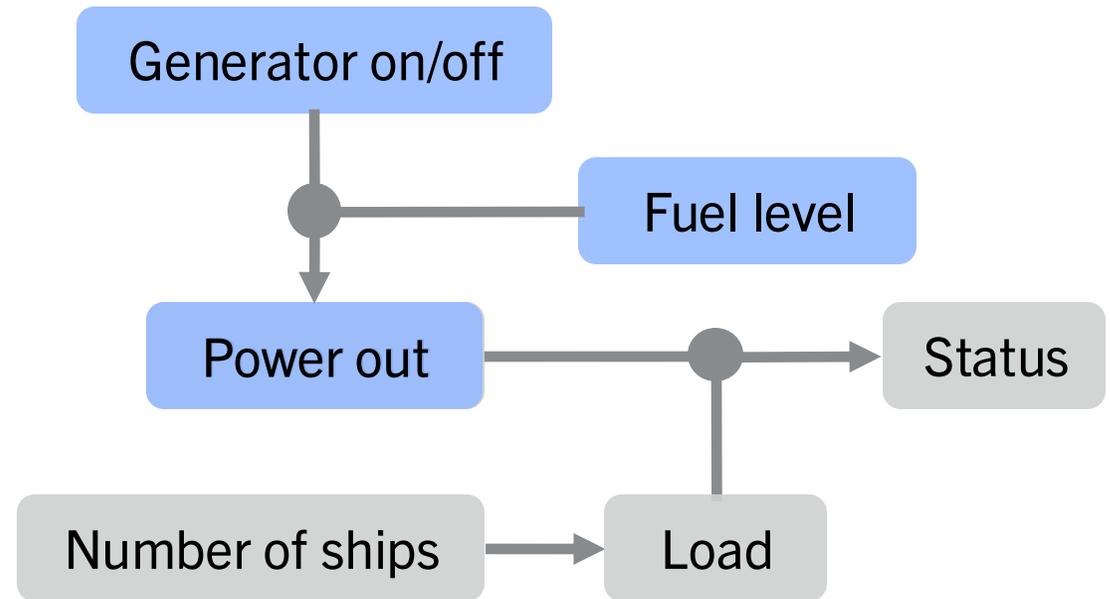
Composable with other graphs along shared nodes (union)

All simulation paths remain consistent *if* new scope does not violate behavioral assumptions



Emergent behavior is provided entirely from composition

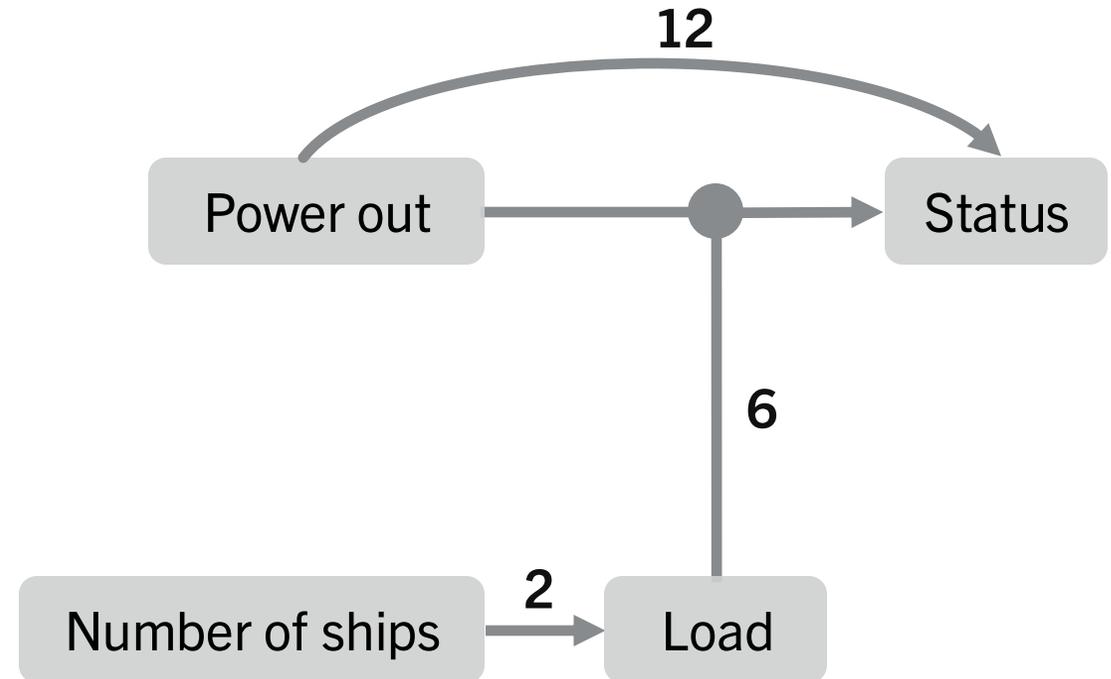
All simulation paths remain consistent *if* new scope does not violate behavioral assumptions



Weights allow model characterization

Edge labels allow models to be compared (model selection)

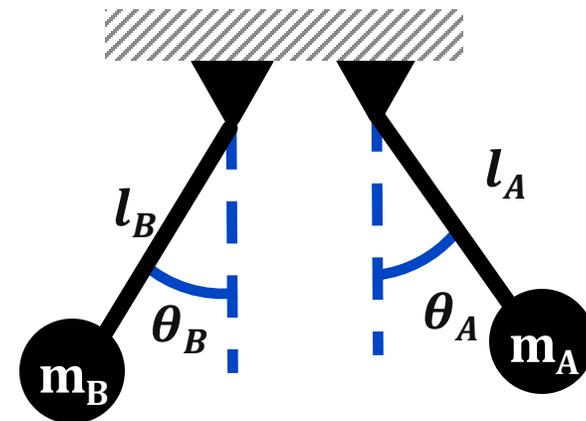
Labels can reference a model's computation time, availability, parallelization, etc.



Emergent behavior arises out of composed functions

$$\ddot{\theta}_A = -\frac{g}{l_A} \sin \theta_A$$

$$\ddot{\theta}_B = -\frac{g}{l_B} \sin \theta_B$$

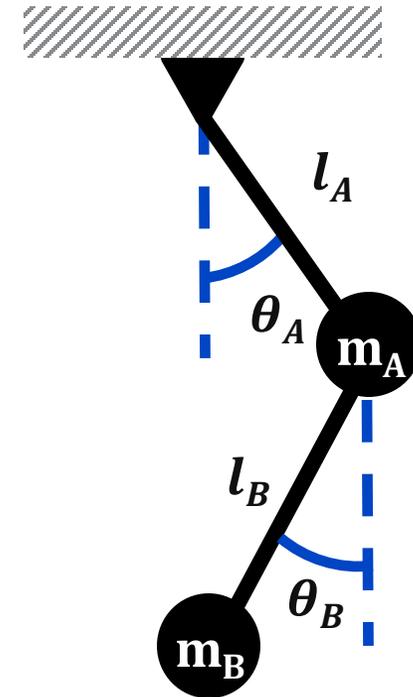


System is fully defined

When the models do not compose, the emergent behavior is not provided

$$\ddot{\theta}_A = -\frac{g}{l_A} \sin \theta_A$$

$$\ddot{\theta}_B = -\frac{g}{l_B} \sin \theta_B$$

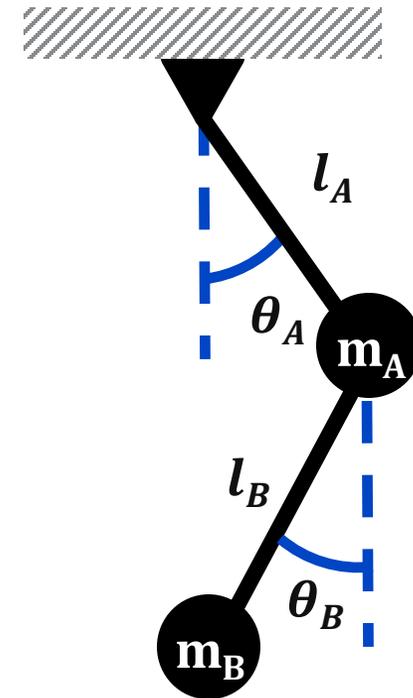


System cannot be represented as desired with the given nodes

Composition must be provided by showing the relationships between nodes

$$\ddot{\theta}_A = -\frac{g}{l_A} \sin \theta_A$$

$$\ddot{\theta}_B = -\frac{1}{l_B} (\ddot{x}_B \cos \theta_B + \sin \theta_B (\ddot{y}_B + g))$$



New model shows how the pendulums can be joined

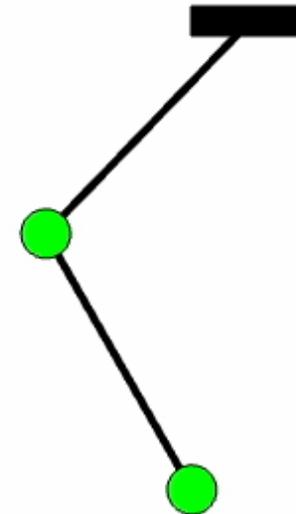
When composition is given, the emergent behavior can be fully realized

$$\ddot{\theta}_B = -\frac{1}{l_B} (\ddot{x}_B \cos \theta_B + \sin \theta_B (\ddot{y}_B + g))$$

where:

$$\ddot{x}_B = l_A (\alpha_A \cos \theta_A - \omega_A^2 \sin \theta_A)$$

$$\ddot{y}_B = l_A (\alpha_A \sin \theta_A + \omega_A^2 \cos \theta_A)$$



Solving for \ddot{x}_B and \ddot{y}_B using terms from the graph for A gives you the emergent behavior