



CAMBRIDGE  
**CARES**

CAMBRIDGE CENTRE  
FOR ADVANCED RESEARCH AND  
EDUCATION IN SINGAPORE LTD.



**Prof Markus Kraft**  
CARES Director

Digital Transformation

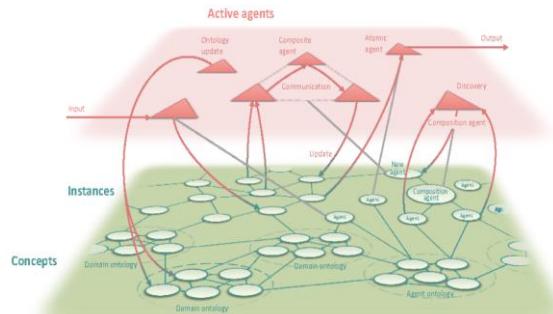
# Ten Years of Digital Transformation at CARES

C4T answers the question of how to positively contribute to Singapore's ratification of the Paris Agreement on climate change while ensuring the country's progress and prowess in economic, technological, environmental and social dimensions.



- **IRP 1: Sustainable reaction engineering** for carbon neutral industry
- **IRP 2: Electrosynthetic pathways** for advanced low-carbon chemical manufacturing
- **IRP 3: Combustion** for cleaner fuels and better catalysts
- **IRP 4: Better, cleaner heat usage**  
**IRP BB: Better business – pathways to industrial decarbonisation**
- **IRP JPS: The J-Park Simulator**

# Ten Years of Digital Transformation at CARES



**J-Park Simulator**, under **C4T** Cambridge Centre for Carbon Reduction in Chemical Technology



**PIPS**, From Digital Twins to Real Time AI-supported Plant Operation



**Cooling Singapore**, exploring heat effects of industry, buildings and transport in Singapore



**eCO<sub>2</sub>EP**, developing ways of transforming CO<sub>2</sub> from industrial processes into useful compounds (*completed*)



**Cities Knowledge Graph**, dynamic KG for district heating networks (*completed*)

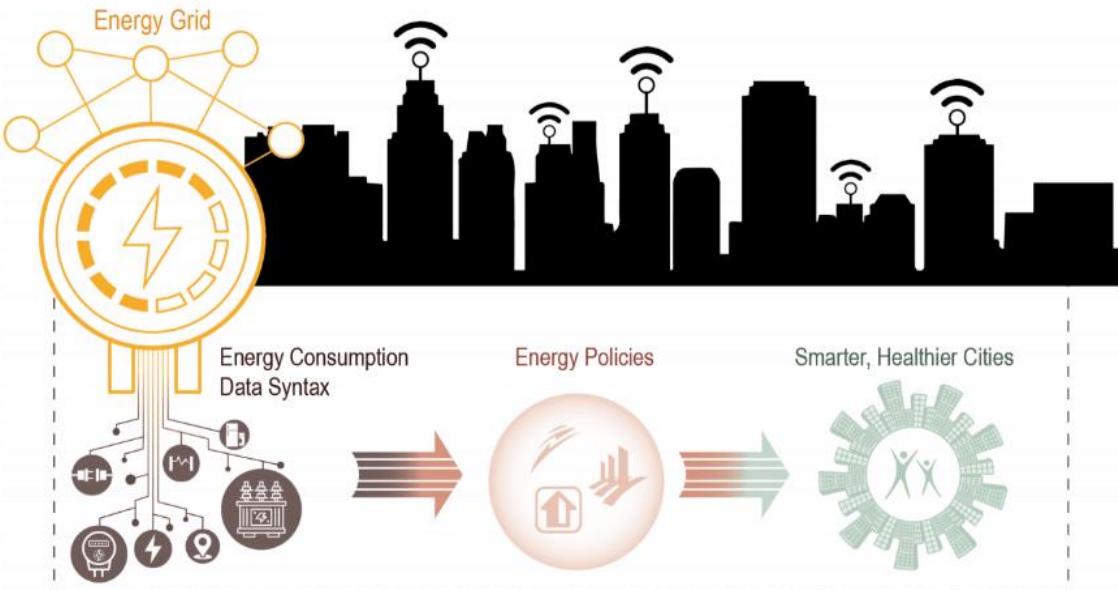


**CEUS**, Consumer Energy Usage Data in Smart City Development (*completed*)

# Ten Years of Digital Transformation at CARES

## Consumer Energy Usage Data in Smart City Development (CEUS)

CEUS aims to lay the groundwork for Singapore consumers to manage their energy usage beyond that of utility bill collection.



### Technology development

- Integrated the data into a knowledge graph for City Information Modelling
- CEUS laid the groundwork for a **Singapore-specific Common Information Model (CIM) grammar** to standardise the representation of consumer energy data

### Anticipated impacts

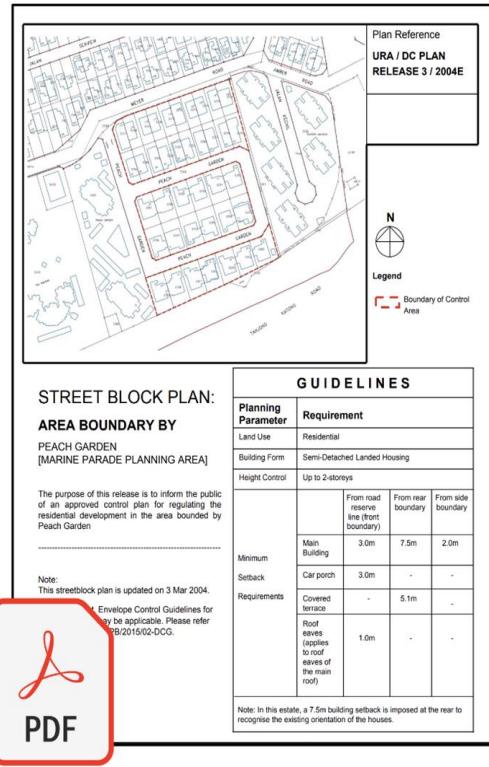
- Consumers could enjoy lower utility bills, select suitable retail electricity offerings, and harness renewable energy
- Building level energy consumption and costs could reduce
- Enhance grid resilience

# Ten Years of Digital Transformation at CARES

## Cities Knowledge Graph (CKG)

Transforming **master-planning related data, information and knowledge** into a semantic and extensible platform – a **knowledge graph**. This would benefit urban planning and support policy makers to map future targets.

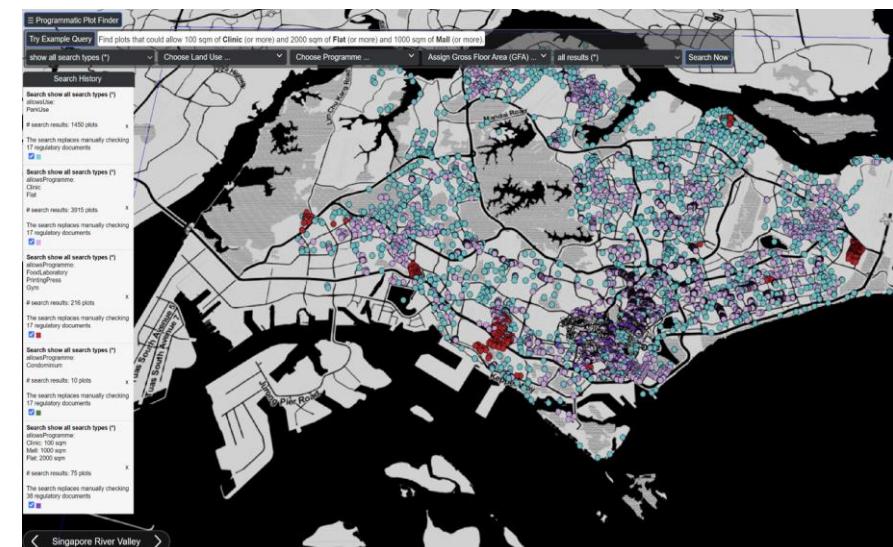
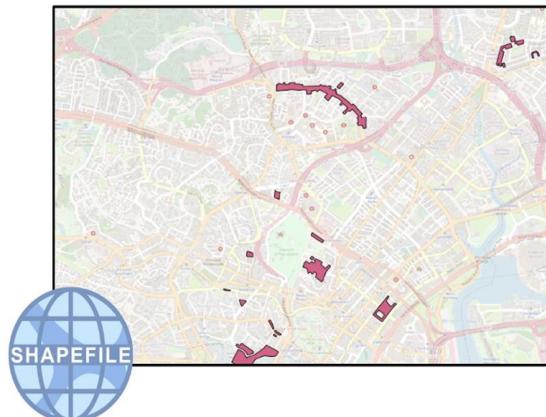
PDF documents



Online text and iconography



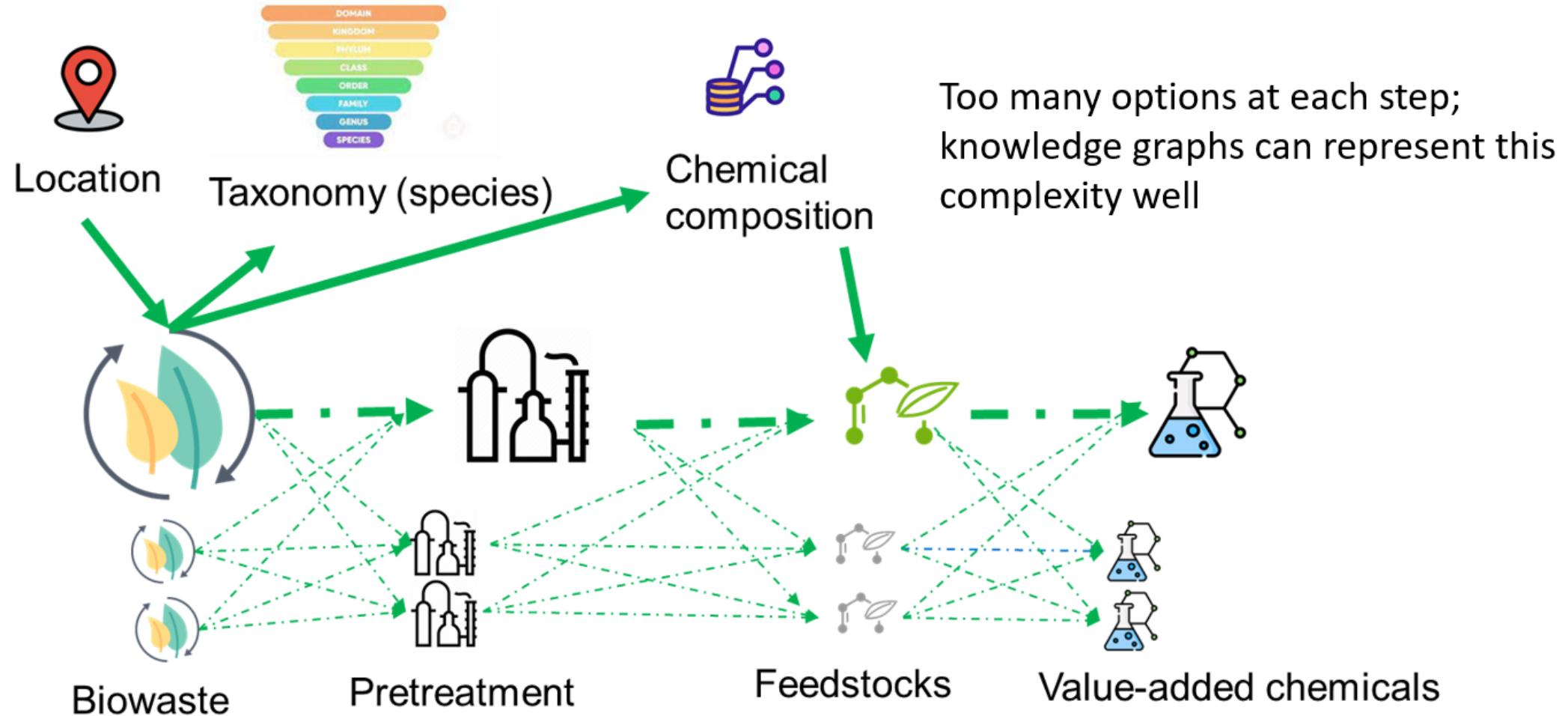
GIS layer (data.gov.sg)



# Ten Years of Digital Transformation at CARES

Knowledge graphs for the biowaste-to-chemicals domain

What are the **most sustainable routes** from **biowaste** to **value added chemicals** and **how can we find them?**

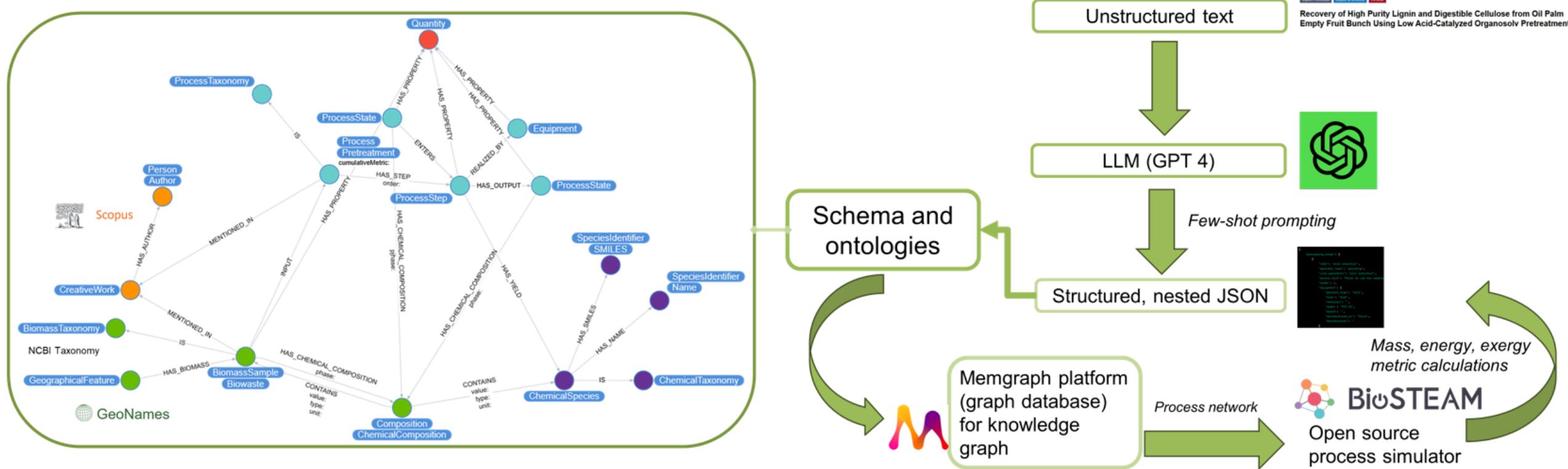


# Ten Years of Digital Transformation at CARES

Knowledge graphs for the biowaste-to-chemicals domain

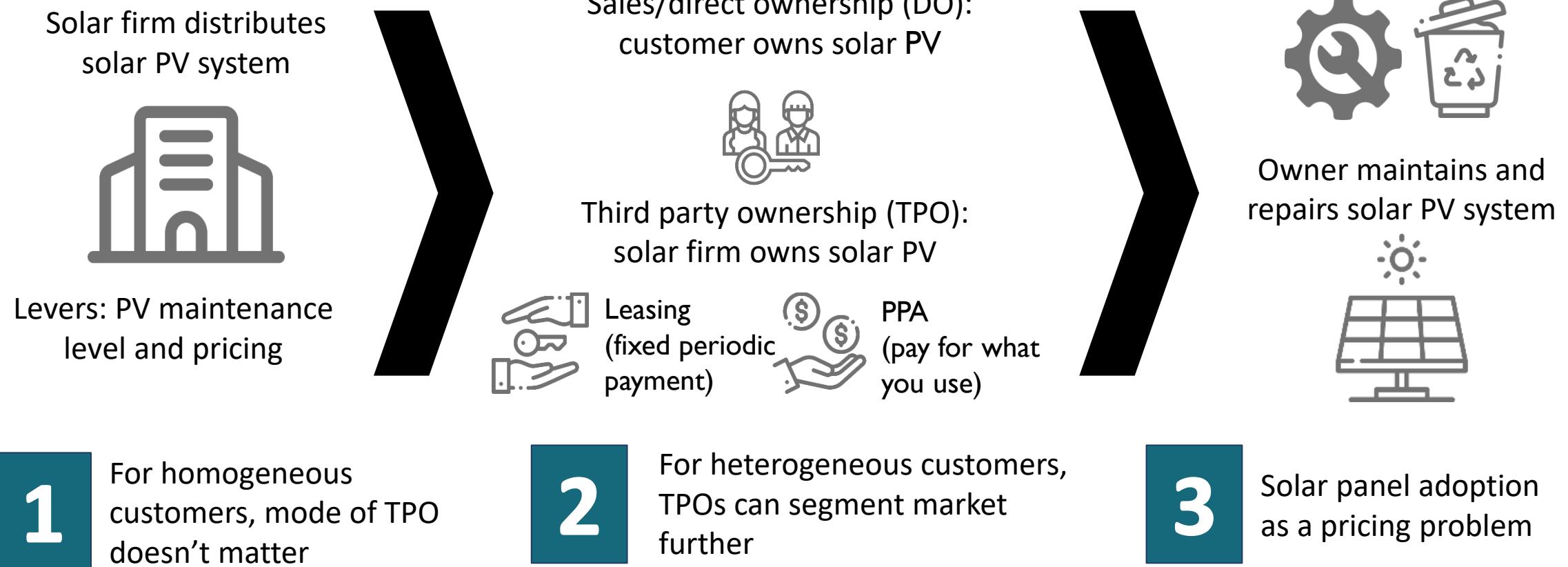
What are the **most sustainable routes** from **biowaste** to **value added chemicals** and **how can we find them?**

## Workflow for knowledge graph population



# Ten Years of Digital Transformation at CARES

## Incentivizing Solar Panel Adoption

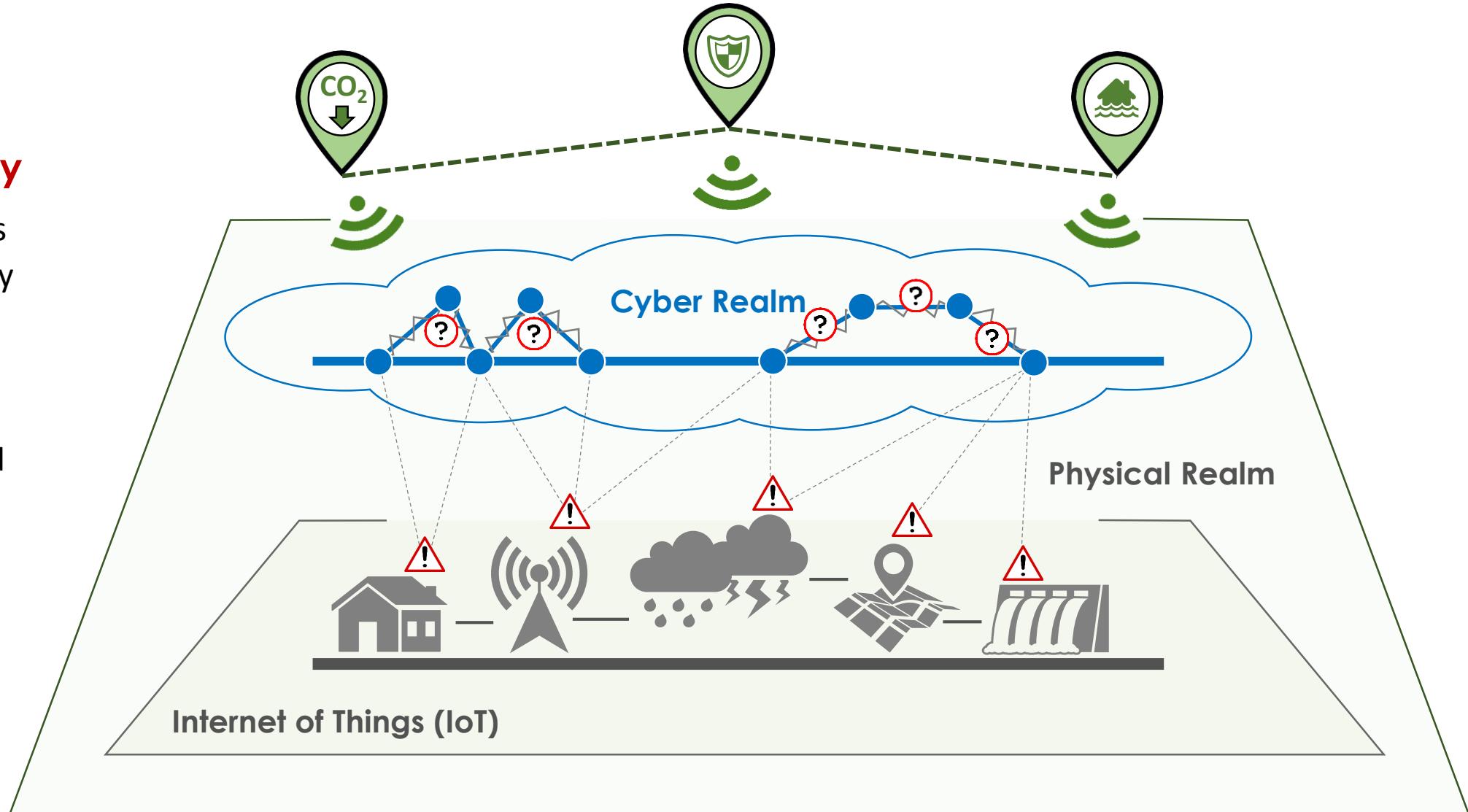


Building on product-as-service models for clean technologies, we can leverage data-driven approaches to generate further market insights

# The Problem

## ⚠️ Low Interoperability

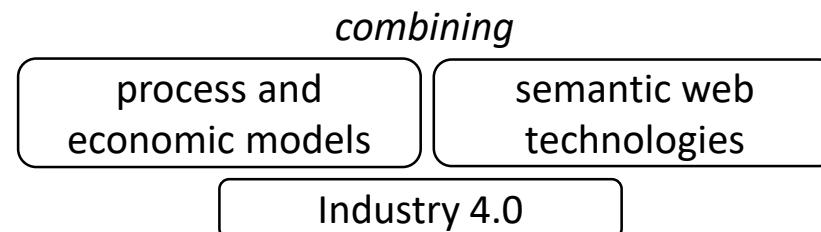
- Different protocols and data ambiguity
- High friction in exchange and integration
- Lock-in effects and surging switching cost



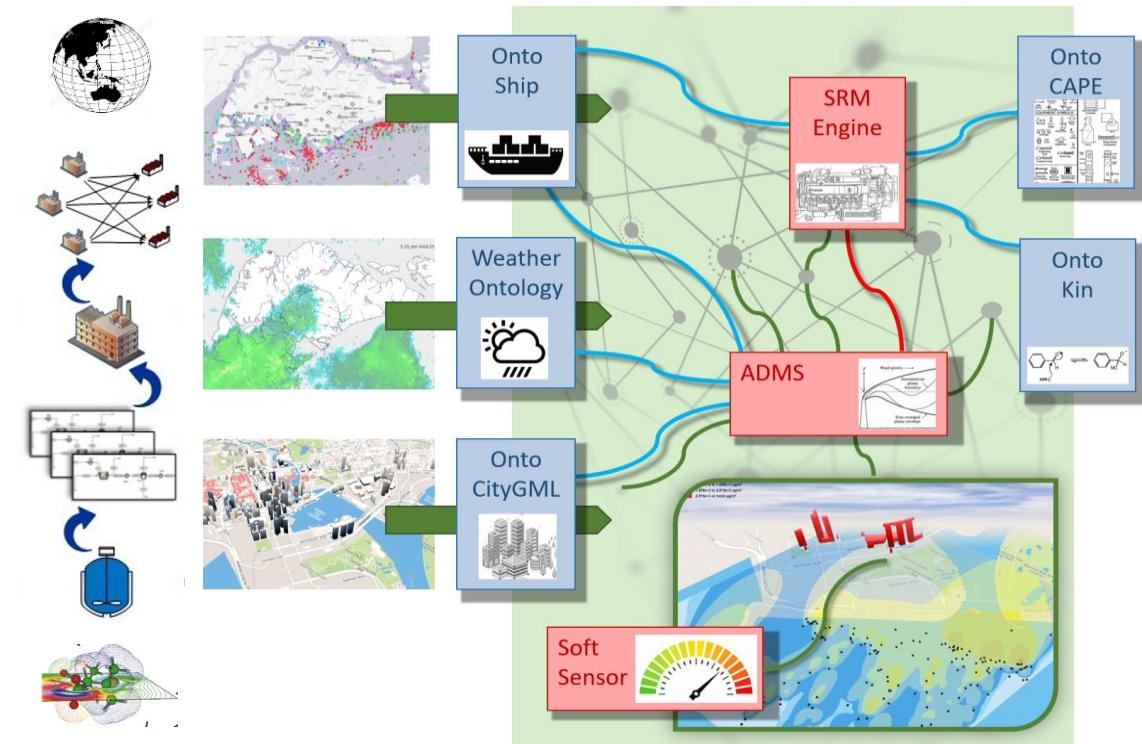
# Ten Years of Digital Transformation at CARES

J-Park Simulator (JPS) – an interdisciplinary research programme within C4T

Creating an architecture for a ***universal digital twin*** – something that can describe the state and behaviour of any interconnected system.

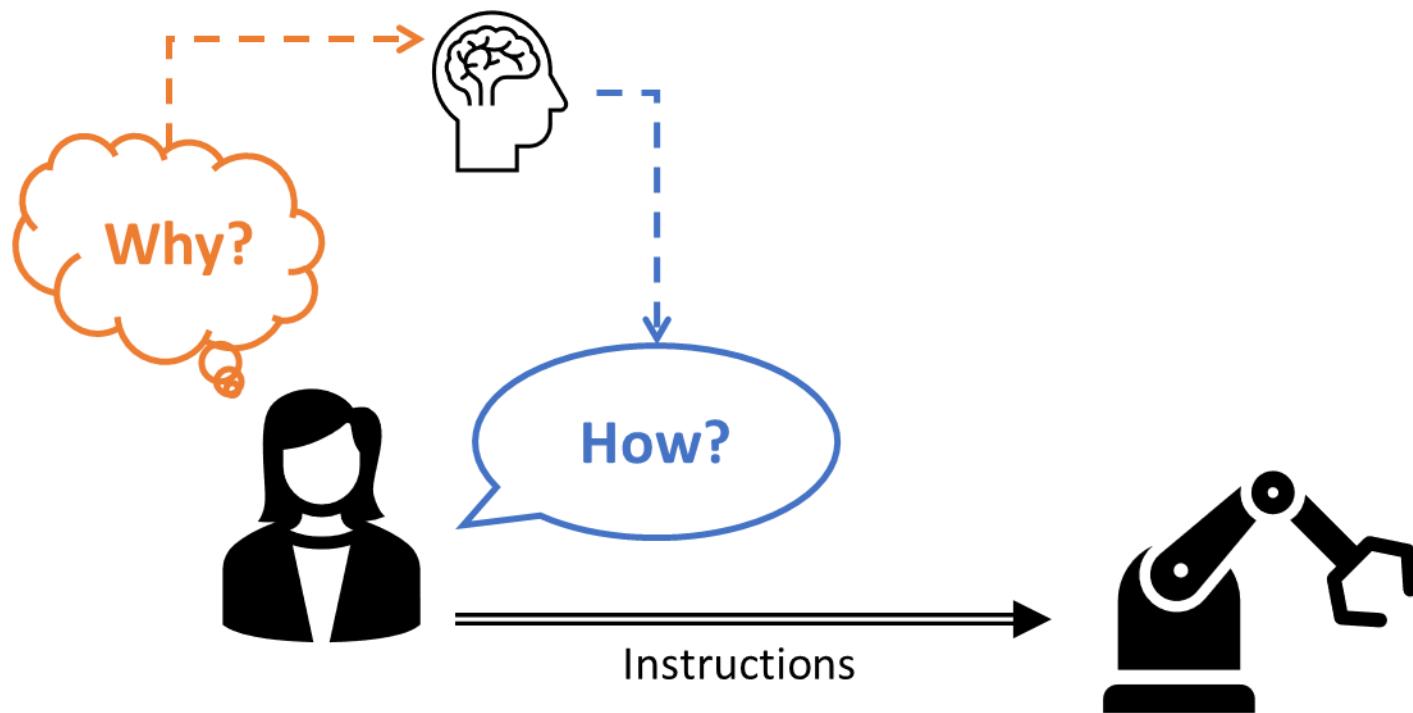


- JPS sets the benchmark for The World Avatar**
- JPS successfully estimated the total yearly emissions from Jurong Island (29MTCO<sub>2</sub>) in C4T Phase 1
  - The World Avatar raises the bar and aims to create a digital avatar of the real world – an all-encompassing world model.

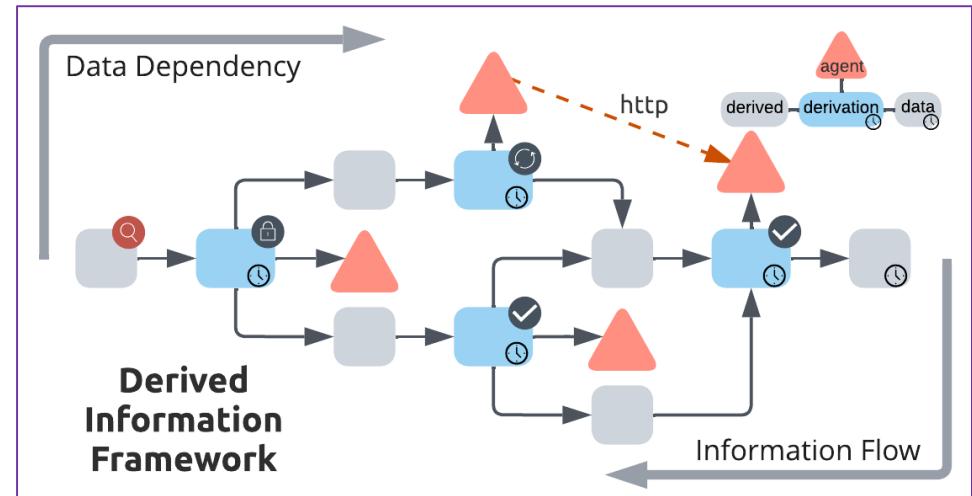
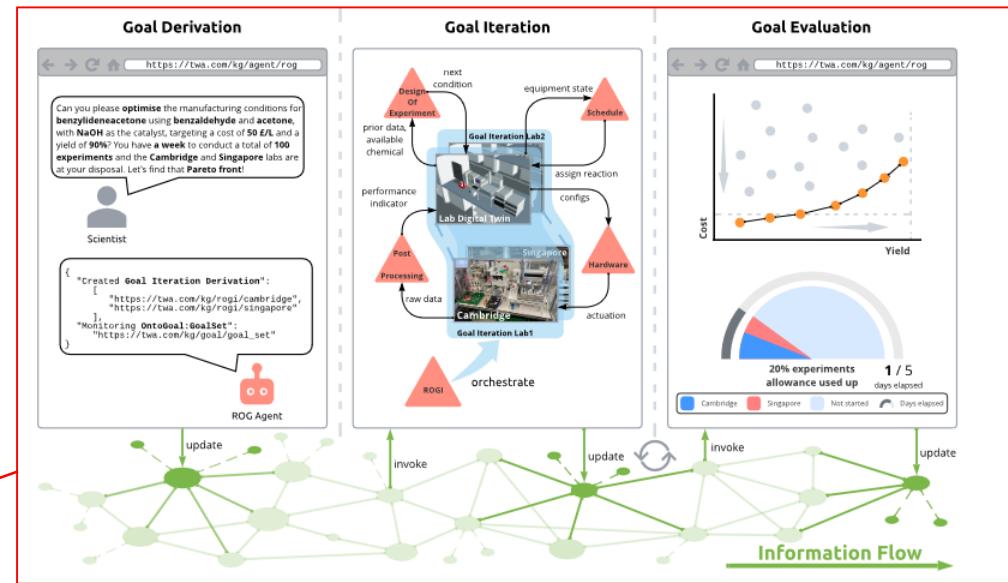
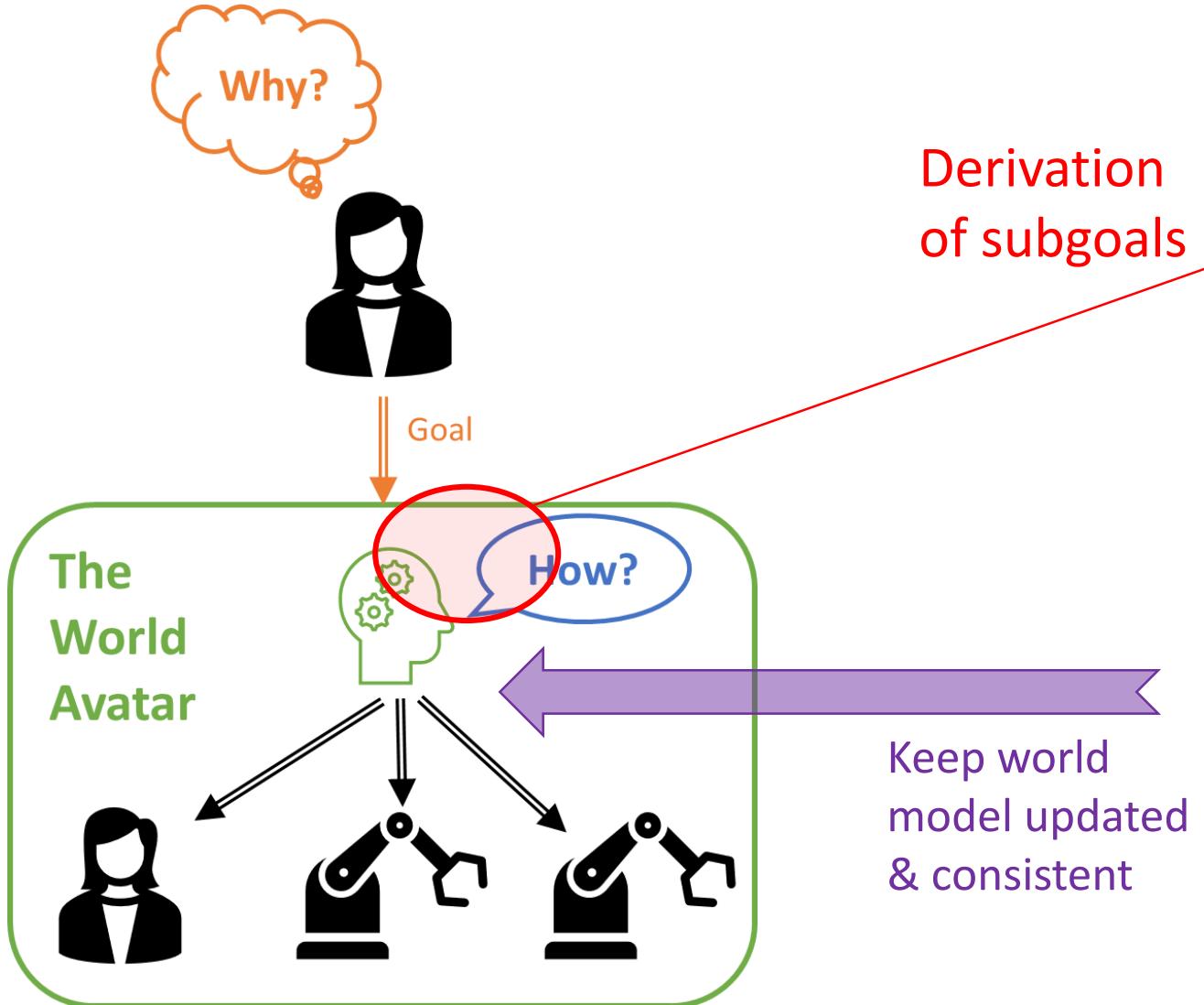


A change in  
perspective

# Human-in-the-loop – so far...



# Human-in-the-loop - TWA



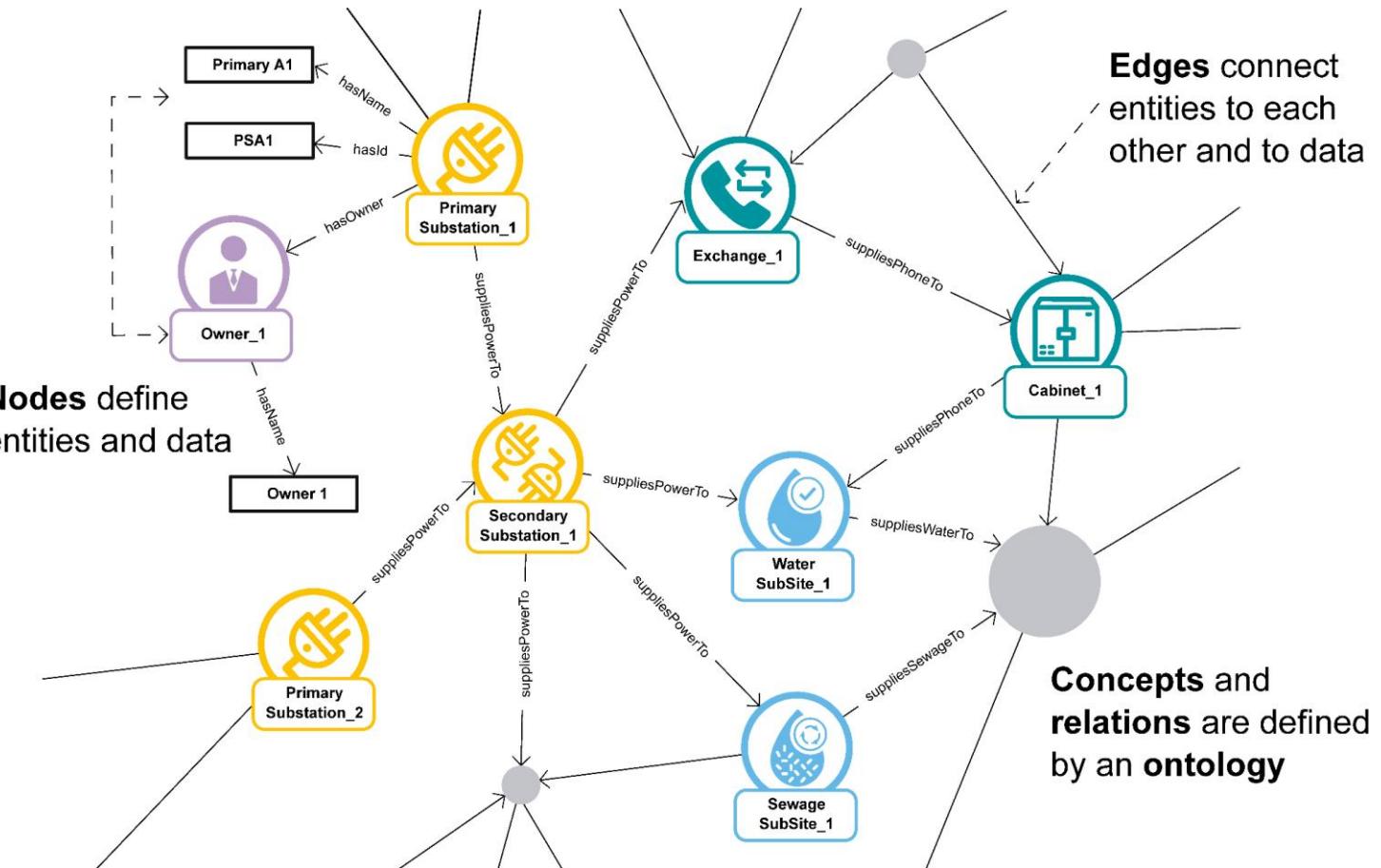
# The Proposed Solution

- **Ontologies** express **conceptual models** of particular domains
- Using ontologies to represent data in logical **knowledge graphs** (KGs)
- Distributed over the internet using semantic web technology



SOURCE:

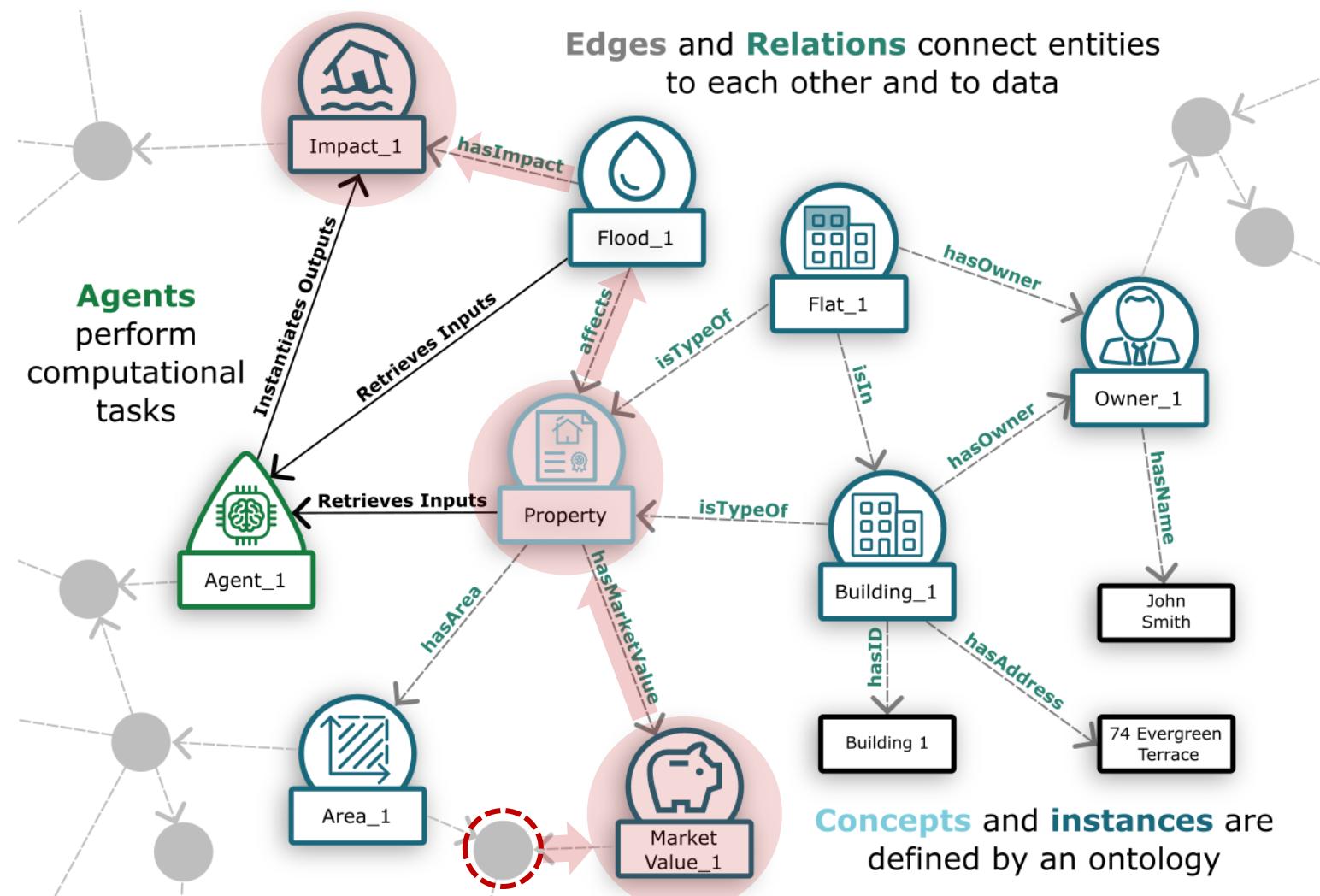
[https://commons.wikimedia.org/wiki/File:FAIR\\_data\\_principles.jpg](https://commons.wikimedia.org/wiki/File:FAIR_data_principles.jpg)



SOURCE: <https://digitaltwinhub.co.uk/credo/>

# The Proposed Solution

- **Ontologies** express **conceptual models** of particular domains
- Using ontologies to represent data in logical **knowledge graphs** (KGs)
- Distributed over the internet using semantic web technology
- **Automated cascading** of new information through entire KG based on dependencies



# The World Avatar (TWA)

A domain-agnostic dynamic Knowledge Graph approach



## THE WORLD AVATAR

An open digital ecosystem that unlocks the power of data  
and knowledge



### Connect

Break down silos and utilise semantic knowledge graphs to unlock the power of your organisation's data



### Control

Utilise data-supported decision intelligence to discover and implement value-adding changes in the physical world



### Query

Reveal insights through analytics and visualisation to better understand the landscape you operate in



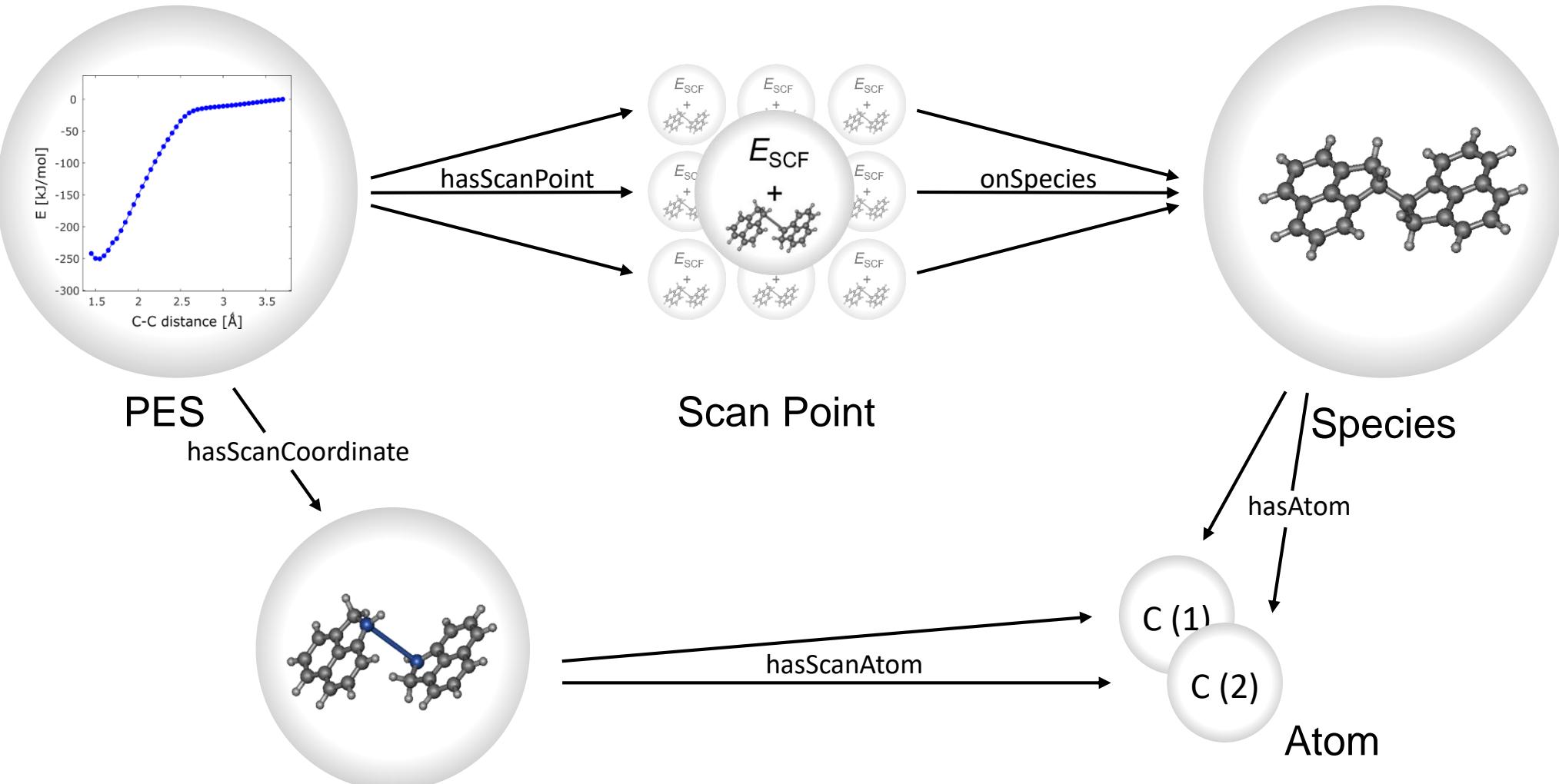
### Imagine

Explore parallel-world scenarios to safely predict and explore the real-world impacts of changes and decisions

# Any Scale

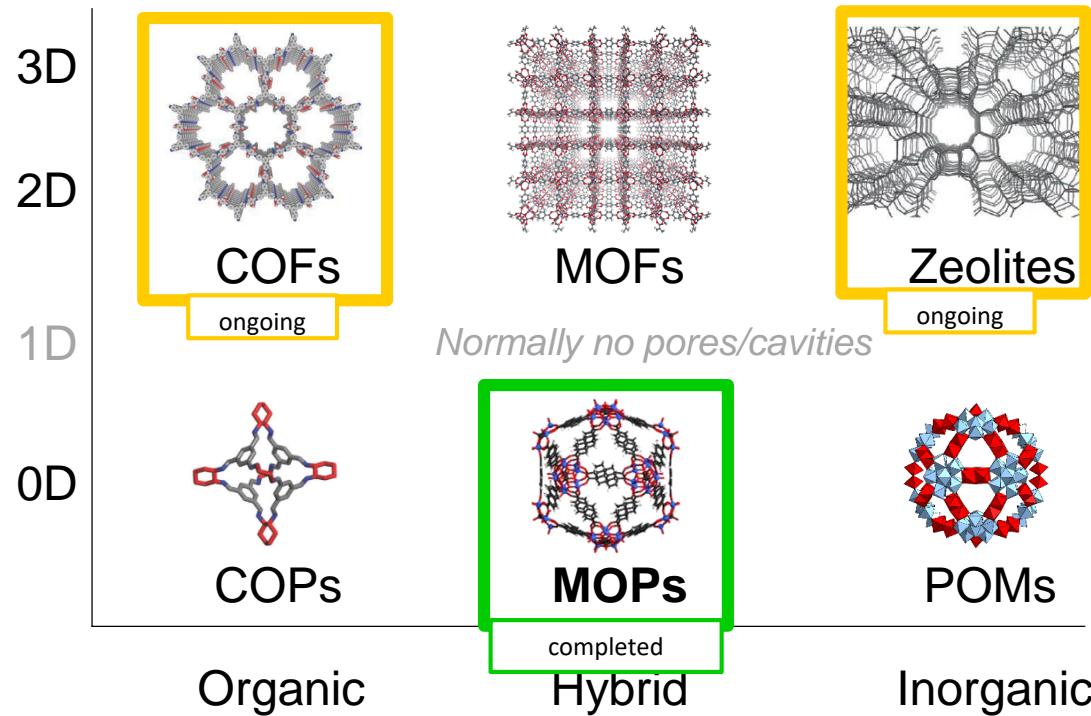
# The World Avatar (TWA)

## Automated atomistic understanding



# The World Avatar (TWA)

## Automated derivation of high value materials

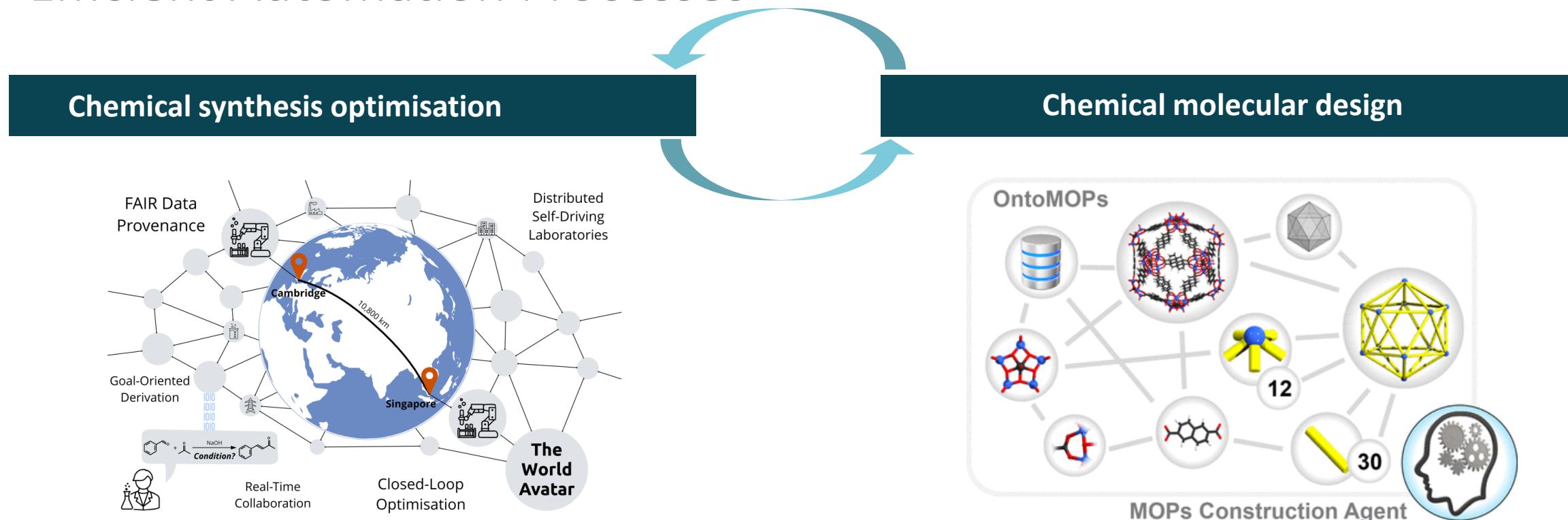


- Materials are made of chemical building units (CBUs).
- By changing CBUs, one can rationally design and synthesize a plethora of new materials with tailoring porosity/cavity sizes, electronic structure and chemical properties.

# The World Avatar (TWA)

## Efficient Automation Processes

Scale - Molecular

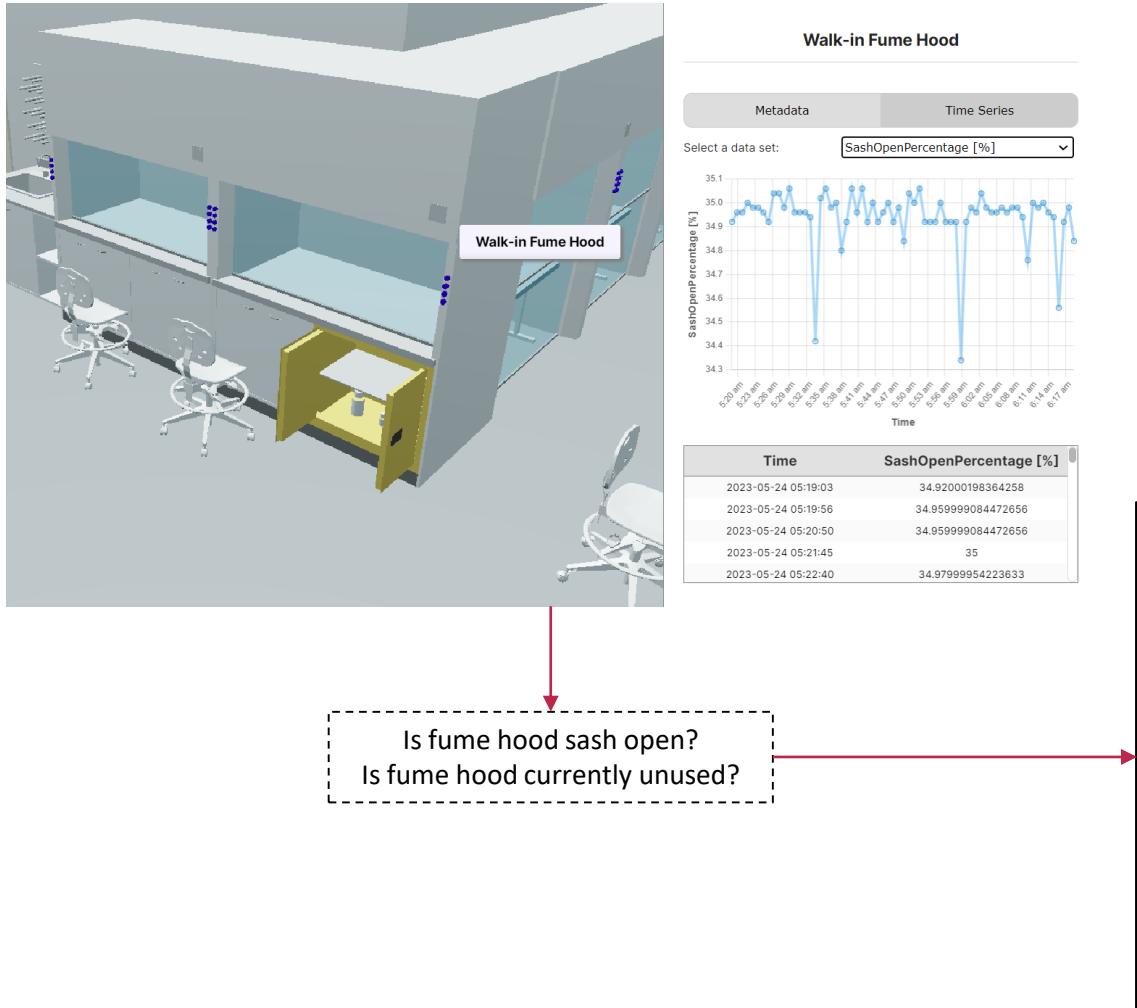


The discovery agent enables scientists to launch an autonomous workflow by specifying a goal request, which activates the knowledge graph's dynamic information flow throughout the experimentation process

Using rational design principles, and automation framework from TWA, the discovery agent synthesised a novel library of 1418 Metal–Organic Polyhedras (MOPs) with structural diversity and tunability for targeted drug delivery applications

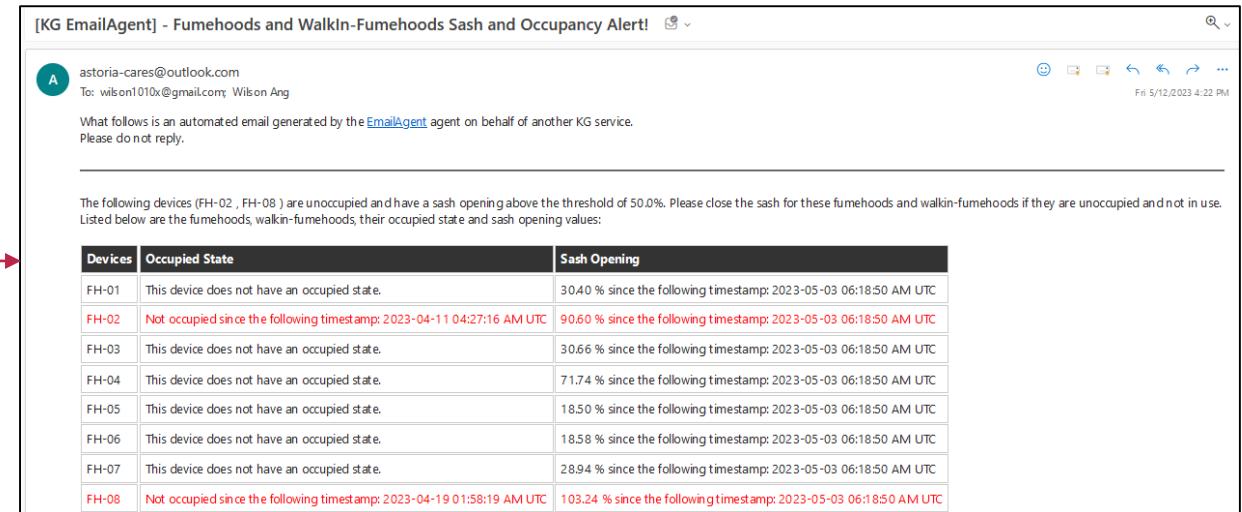
# The World Avatar (TWA)

## Augmented CARES Lab



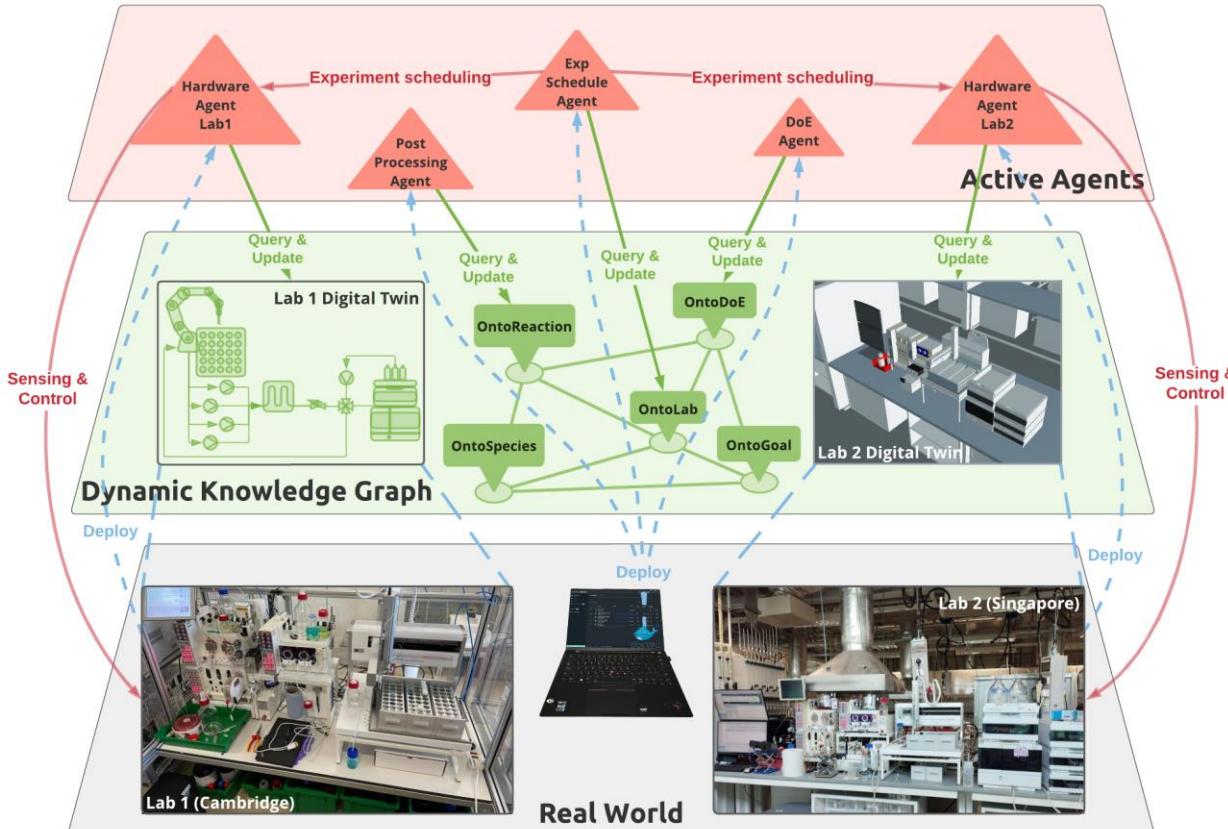
## Energy Savings

- The CARES Lab digital twin integrates live data from various equipment with their BIM representation, in order to create an interoperable system to monitor the energy consumption of the lab devices, along with suggesting and implementing measures to reduce this usage



# The World Avatar (TWA)

## Augmented CARES Lab



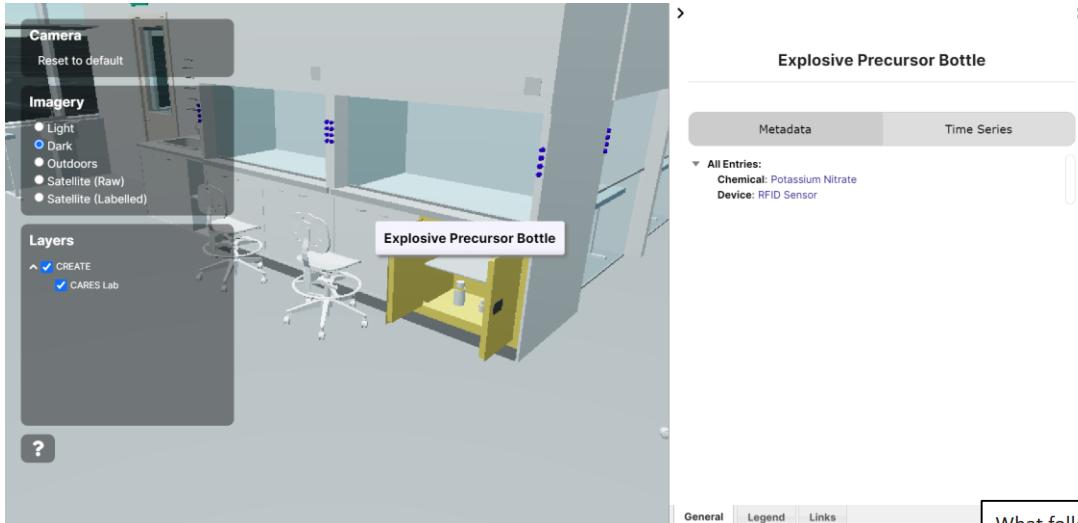
## Experiments

- Using the knowledge graph, a distributed network of self-driving laboratories for flow chemistry was set up and run
- Two robotic setups in Cambridge and Singapore were linked to achieve a collaborative closed-loop optimisation for an aldol condensation reaction in real time
- The framework successfully generates the Pareto front for the yield-cost optimisation problem

Indication of Scale – Building

# The World Avatar (TWA)

## Augmented CARES Lab



## Asset Tracking

- The CARES Lab digital twin integrates live data from various sensors with their BIM representation, in order to create an interoperable system which allows monitoring of explosive precursors along with automated email notification to the Lab Manager

What follows is an automated email generated by the [EmailAgent](#) agent on behalf of another KG service.  
Please do not reply.

The chemical container with the following information has been removed since 2023-03-08 07:03:19 AM UTC. The container has the following label: chemical container 01 and tag ID: 000000000000A000009727 and it is storing a chemical with the following label: KNO3. The chemical has the following GHS hazard statements:  
 H315 : Causes skin irritation [Warning Skin corrosion/irritation]  
 H319 : Causes serious eye irritation [Warning Serious eye damage/eye irritation]  
 H335 : May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation]  
 H272 : May intensify fire; oxidizer [Danger Oxidizing liquids; Oxidizing solids]

The following meta-data was gathered from the machine triggering this notification:  
 Public IP Address: 131.111.184.3  
 Submission Time: 2023-03-27 07:22:48.0390  
 Hostname: c0ccfc8a329  
 Local IP Address: 172.23.0.2

# The World Avatar (TWA)

## BIM-GIS representation of Pirmasens: House 45

**House 45**

**Metadata**

**All Entries:**

- Current Electricity Consumption: 0.315 [kWh]
- Current Relative Humidity: 84 [%]
- Current Diffuse Horizontal Irradia: 35 [w/sqm]
- Current Time: 2022-12-06 14:00:00+00
- Theoretical Roof PV Area: 98.21 [sqm]
- Building Footprint: 113.48 [sqm]
- Current Theoretical Solar Electricity Generation: 0.81 [kWh]
- Current Cloud Cover: 100 [%]
- Current Rainfall: 0 [mm]

**Available solar panel options**

**1) AXIperfect FXXL WB**

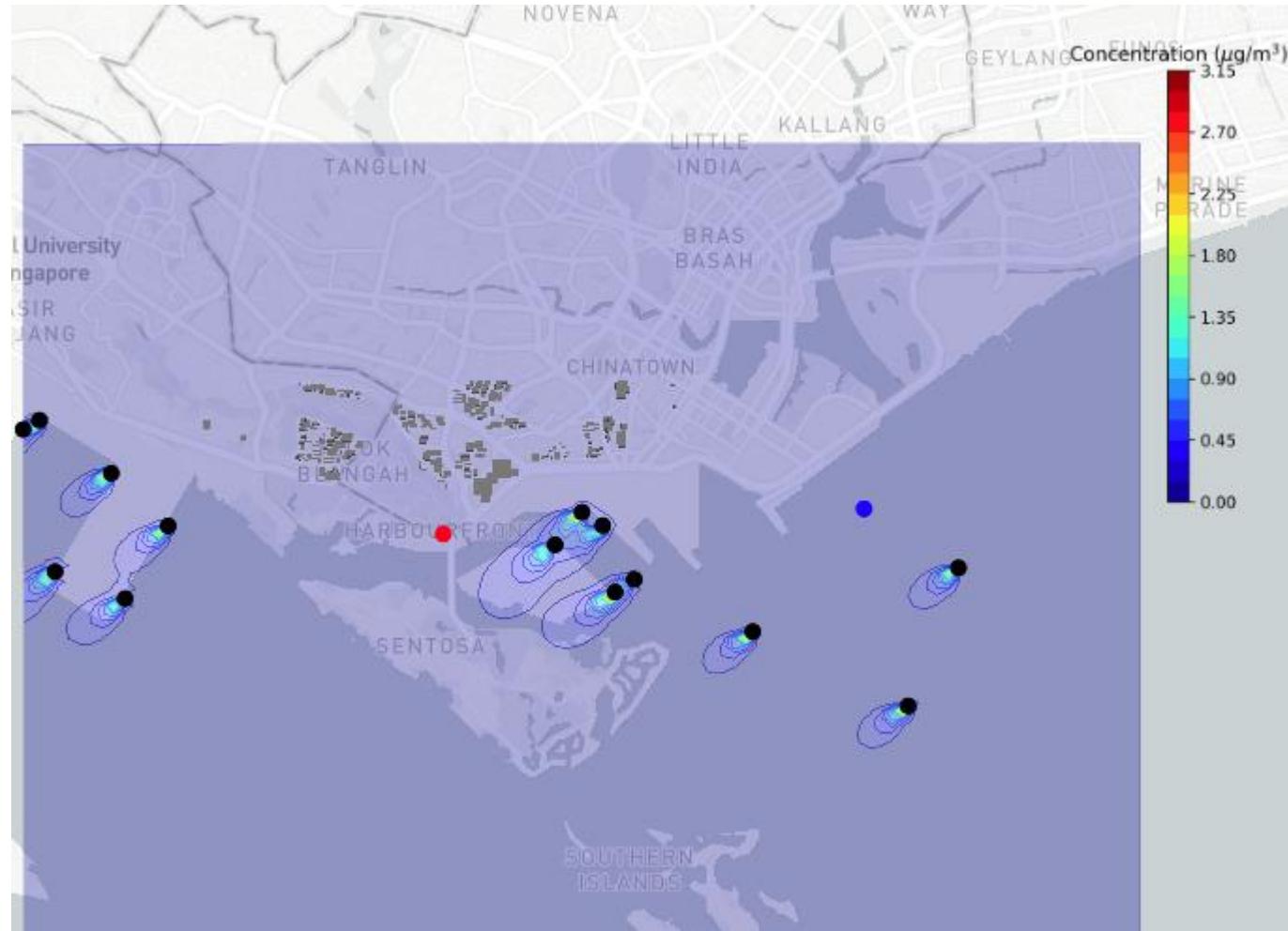
Type: Monocrystalline  
Performance: 415 - 430 Wp  
Panel efficiency: 21.25 ~ 22.02%  
Cost per module: 154€  
Vendor: Axitec Energy  
Dimensions (L x W x H): 1722 × 1134 × 30 mm  
Weight: 21.8kg

General   Legend   Links   [Return](#)

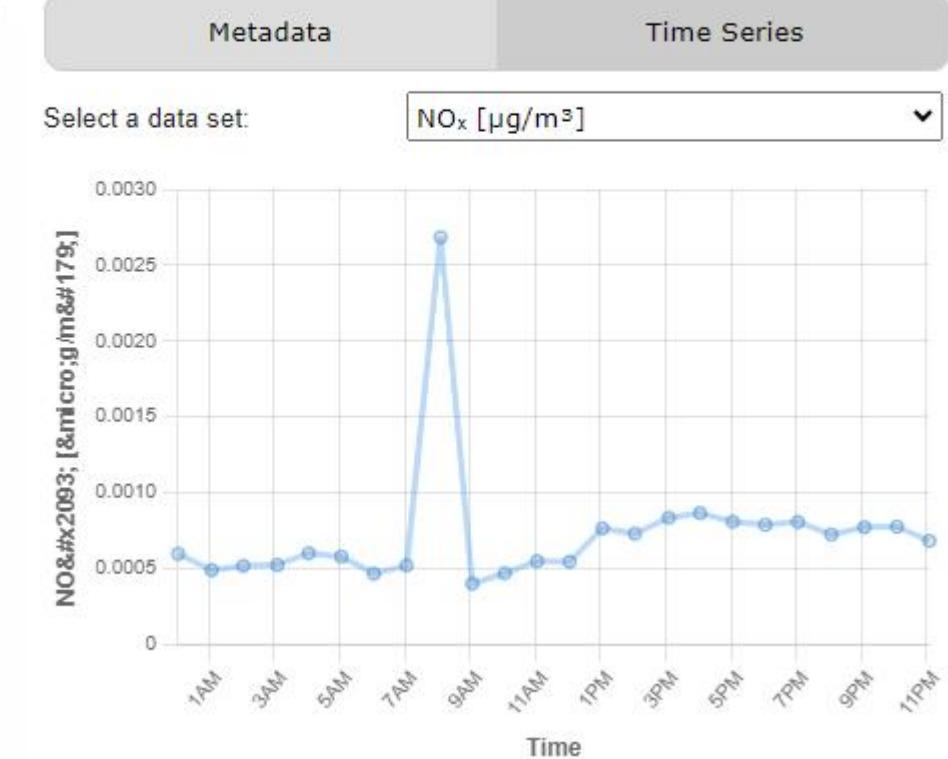
# The World Avatar (TWA)

AERMOD agent: Time evolution of NOx at Harbourfront (red dot)

Scale - City



Virtual sensor



# The World Avatar (TWA)

## Augmenting simulation data with sensor data

- Representation of ambient environmental variables (Noise, Light, Speed) timestamped with coordinates and collected using existing mobile phone sensors, overlayed with estimated ship emissions from an atmospheric dispersion model

Point 1	
Time	Wednesday, 23 November 2022 20:56:01
Latitude	1.281792
Longitude	103.8602
Speed (m/s)	0.999
Light (Lux)	0
Noise (dBFS)	-41
Relative Humidity (%)	76
Temperature (°C)	28.4
UV Index	0
NO <sub>x</sub> (ppb)	< 1 (Good)
O <sub>3</sub> (ppb)	< 1 (Good)
SO <sub>2</sub> (ppb)	< 1 (Good)
PM2.5 (µg/m <sup>3</sup> )	< 1 (Good)
PM10 (µg/m <sup>3</sup> )	< 1 (Good)



# The World Avatar (TWA)

## Augmenting simulation data with sensor data

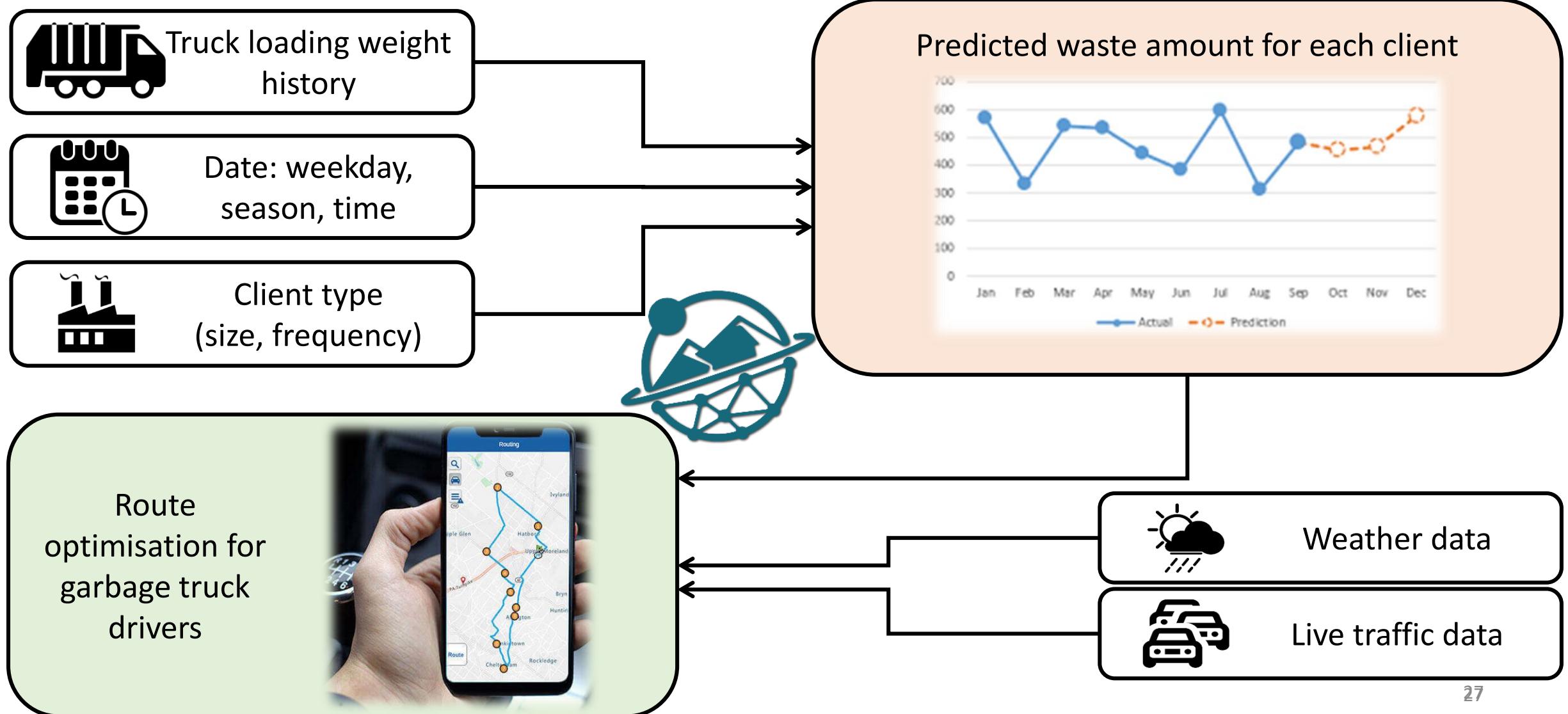
Point 3	
Time	Wednesday, 23 November 2022 21:21:15
Latitude	1.271862
Longitude	103.8639
Speed (m/s)	0.044
Light (Lux)	0
Noise (dBFS)	-160
Relative Humidity (%)	77
Temperature (°C)	28.5
UV Index	0
NO <sub>x</sub> (ppb)	482 (Moderate)
O <sub>3</sub> (ppb)	86 (Unhealthy)
SO <sub>2</sub> (ppb)	84 (Moderate)
PM2.5 (µg/m <sup>3</sup> )	128 (Unhealthy)
PM10 (µg/m <sup>3</sup> )	247 (Unhealthy)



# The World Avatar (TWA)

## Route optimisation for waste collection

Scale - City



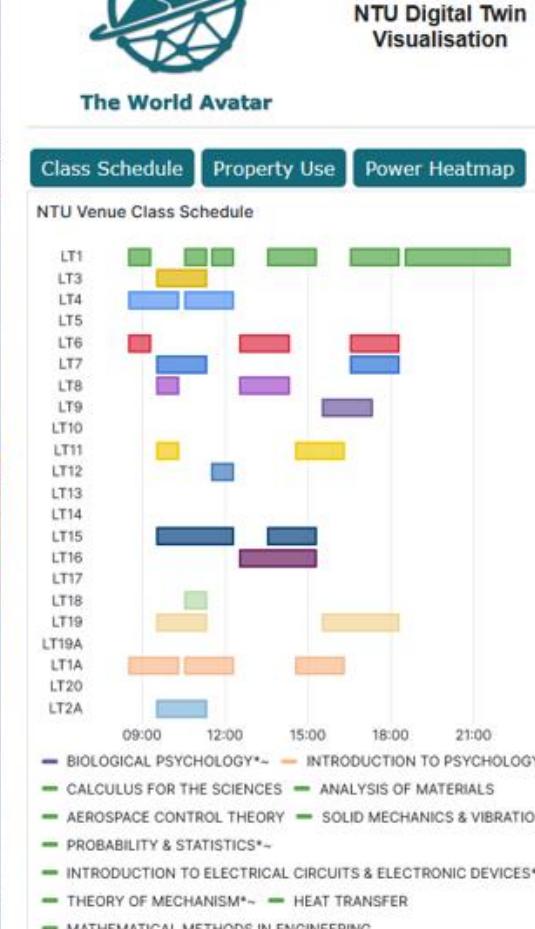
# The World Avatar (TWA) KG-Driven Real-Time Network Operation

A knowledge graph based digital twin of the NTU campus incorporating 3D building data, class schedules, weather, power systems, power load and solar generation.

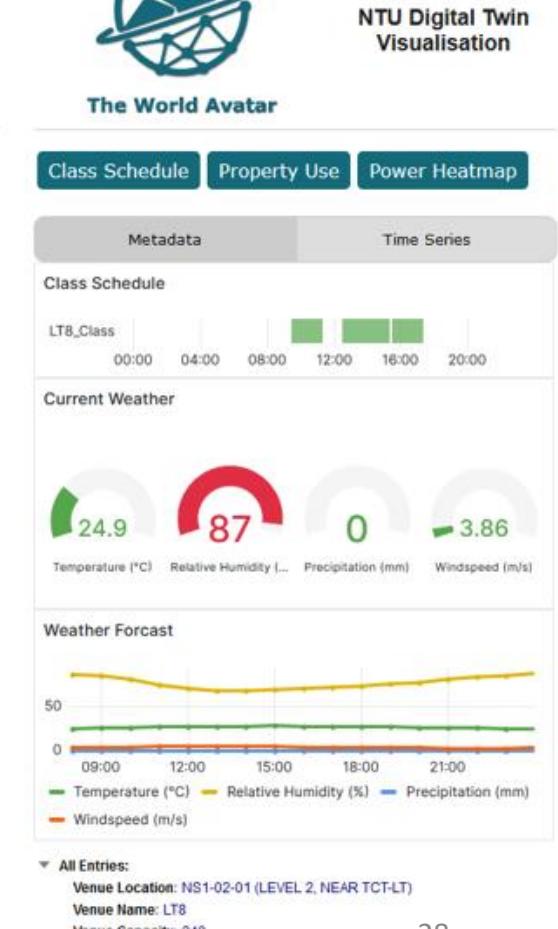
Scale - City



The World Avatar



The World Avatar

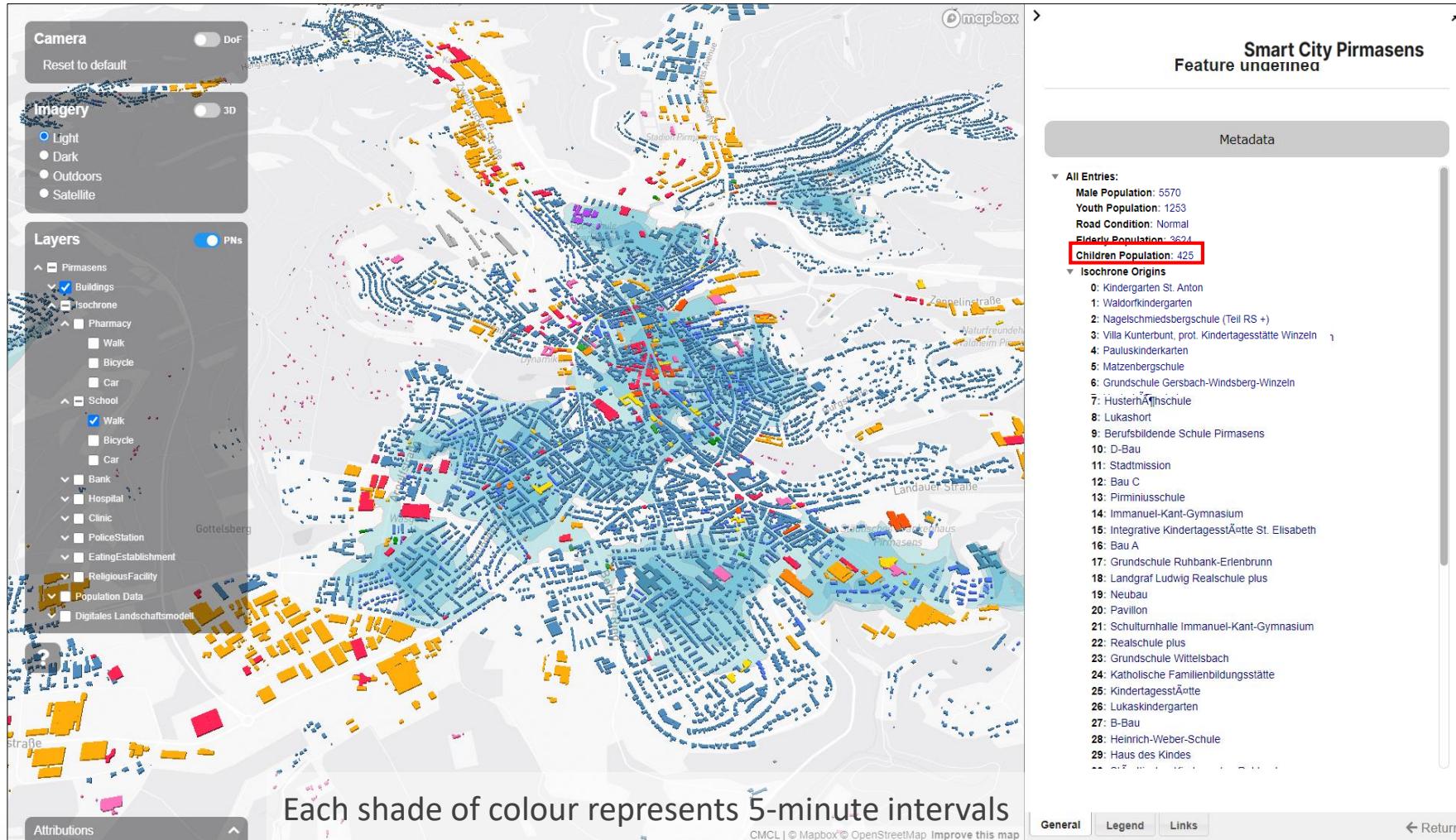


# The World Avatar (TWA) Isochrone map for all schools in Pirmasens

Scale - City



Isochrone map showing coverage of schools within 15 minutes of walking in Pirmasens



Population data from  
Facebook (Meta) – Data  
For Good

Schools in Pirmasens  
from Open Street Map

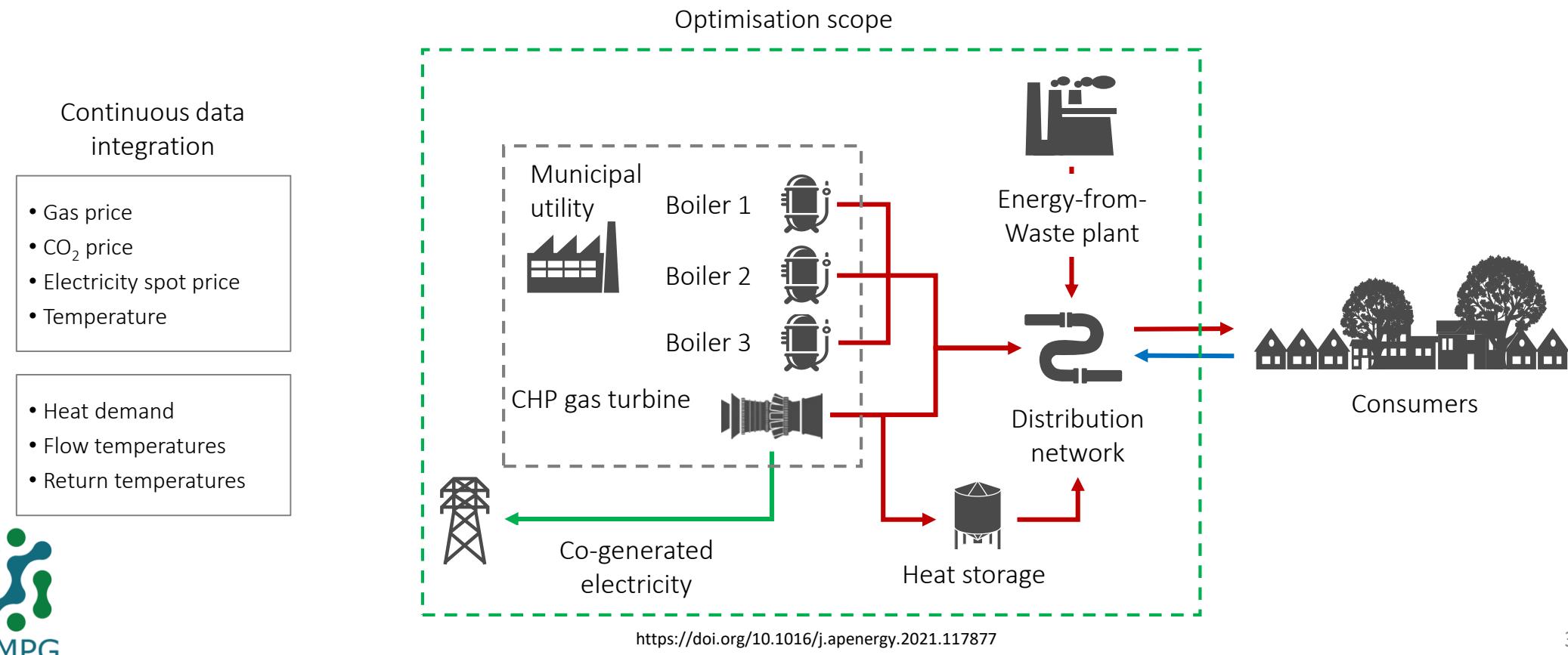
# The World Avatar (TWA)

## Optimal control of a district heating system



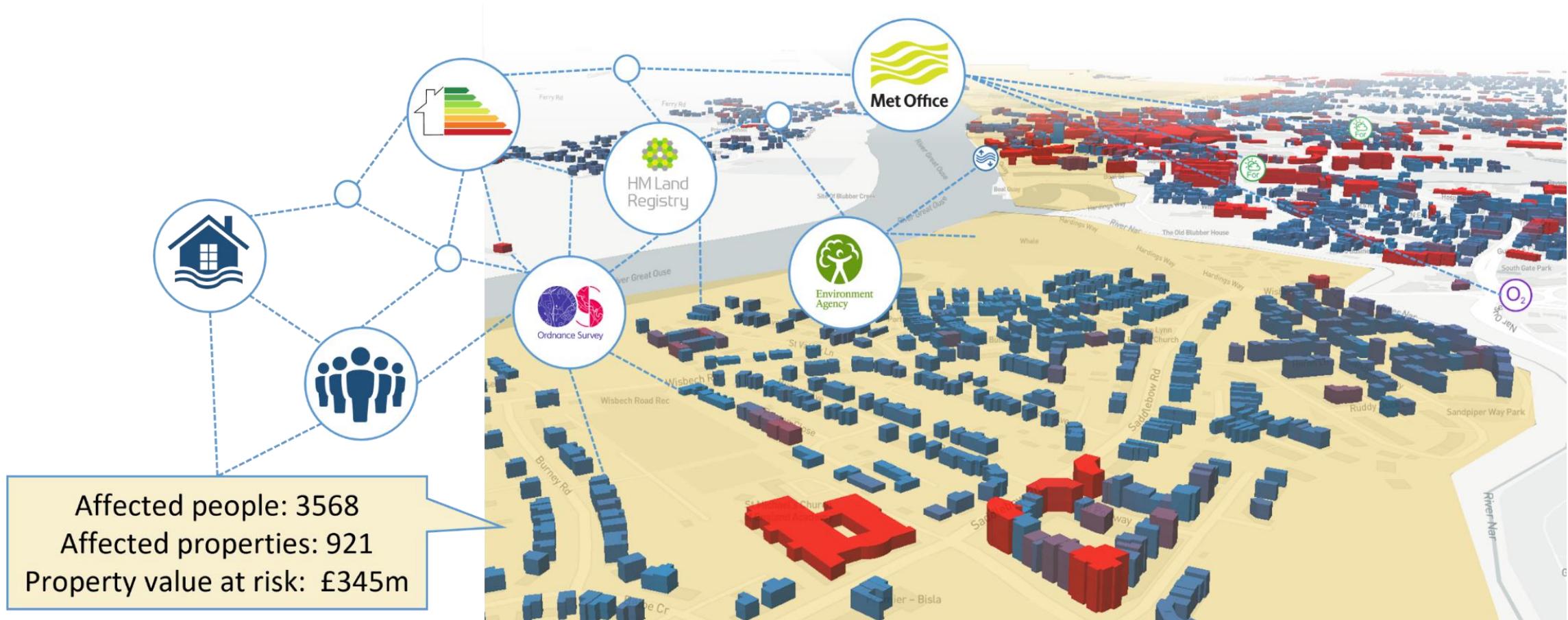
Scale - City

Minimises heat generation cost and optimises the operation of a gas turbine, with continuous data integration and forecast using the knowledge graph



# The World Avatar (TWA)

Representation of cross-domain data in Kings Lynn: Effect of flooding



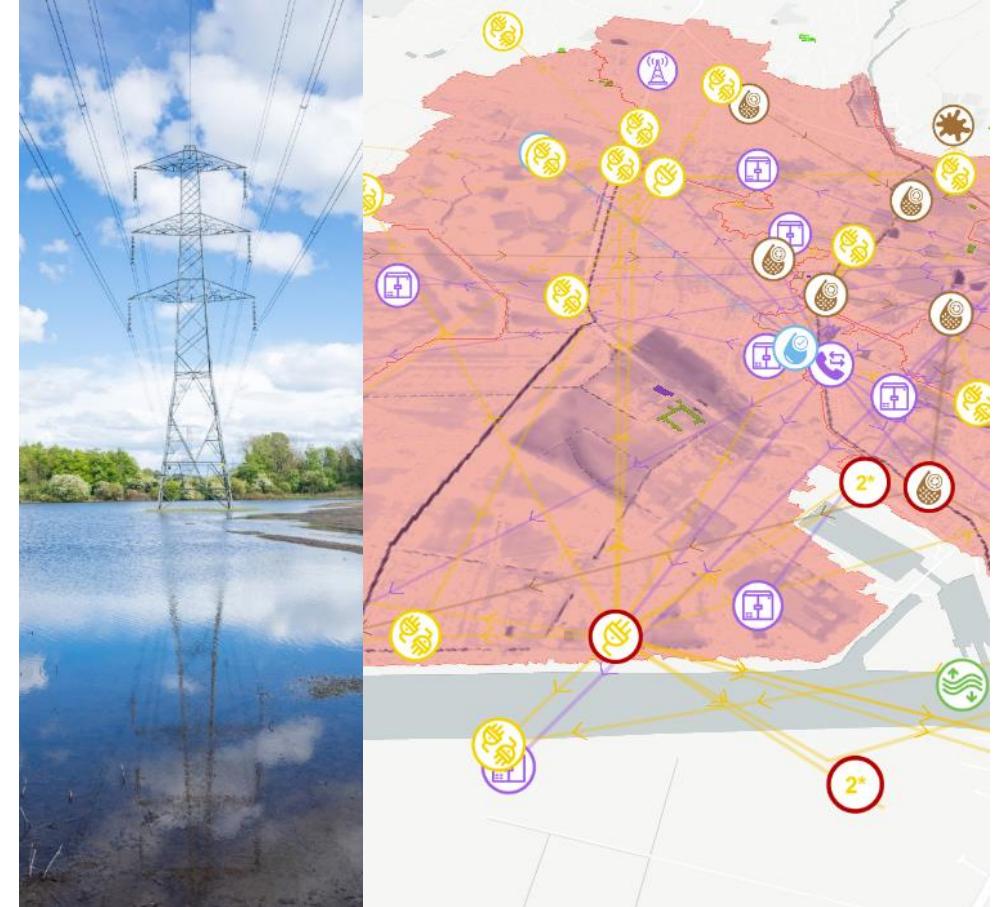
# The World Avatar (TWA) Climate Resilience Demonstrator (CReDo)

Scale - Country



- Critical National Infrastructure is **highly interconnected**.
- The relationships between assets and networks are usually **not known**.
- Resiliency measures can sometimes be **insular**.
- Visualising the interdependencies between sectors enables **collaborative** resilience efforts.

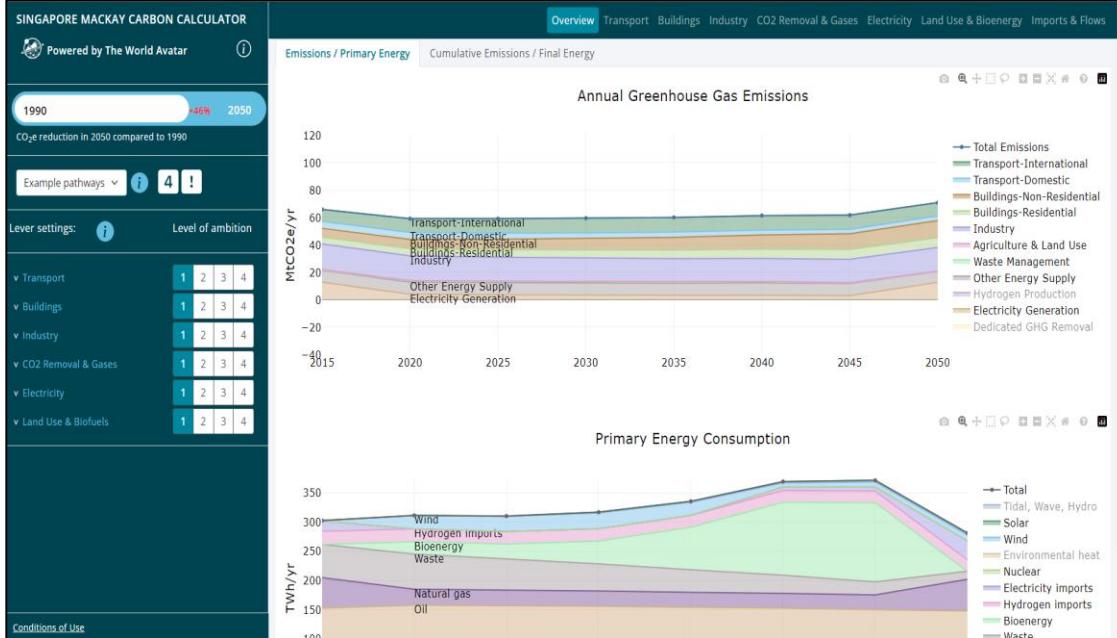
*'Cascading risks—spreading from one Critical National Infrastructure (CNI) sector to another, **magnifying** the impact of an event—were demonstrated vividly by the effects of Storm Arwen in late 2021, which led to **extended** power and communication outages'* - Joint Committee on the National Security Strategy, UK



A real-life flooding event and a simulated example using the CReDo visualisation tool

# The World Avatar (TWA) Singapore MacKay Carbon Calculator

## Detailed calculator



## Lever explanations – Singapore context

**Singapore MacKay Carbon Calculator**

**Buildings: Lighting & Appliances**

This lever controls the sub-levers listed in the table, and ambition levels are for the end year shown on the right-hand side. Units of 'Index' are relative to 2015.

Energy used to provide lighting can be reduced in two ways: reduce the overall demand for lighting, and/or use more efficient lights. Lighting demand could be reduced through improved behaviours and building practices such as turning off unnecessary lights. More efficient lighting options include using Light Emitting Diodes (LEDs). LEDs use half the amount of energy as Compact Fluorescent Lamps (CFLs) and a fifth of that of halogen bulbs. In the calculator, the energy intensity of lighting is the amount of energy consumed by the lighting technology to produce light. Reducing the energy intensity depends on how soon, and to what extent, LEDs can replace existing CFL and halogen bulbs.

Ownership of appliances such as televisions, computers and other goods is increasing, but so too is the efficiency.

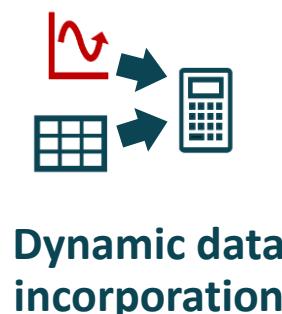
**Key Interaction**

Reducing electricity demand will help reduce energy requirements and emissions from electricity generation.

**Default Timing Start year: 2025, End year: 2050**

Sub-Lever	Units	2015	Level 1	Level 2	Level 3	Level 4
Demand	Index	1.00	1.50	1.00	0.85	0.70
Lighting - Residential	Index	1.00	1.30	1.00	0.75	0.50
Lighting - Non-Res	Index	1.00	1.50	1.00	0.75	0.50
Appliance - Residential	Index	1.00	1.30	1.00	0.90	0.80
Appliance - Non-Res	Index	1.00	1.30	1.00	0.90	0.80

**Residence Appliance - Energy Intensity Index**

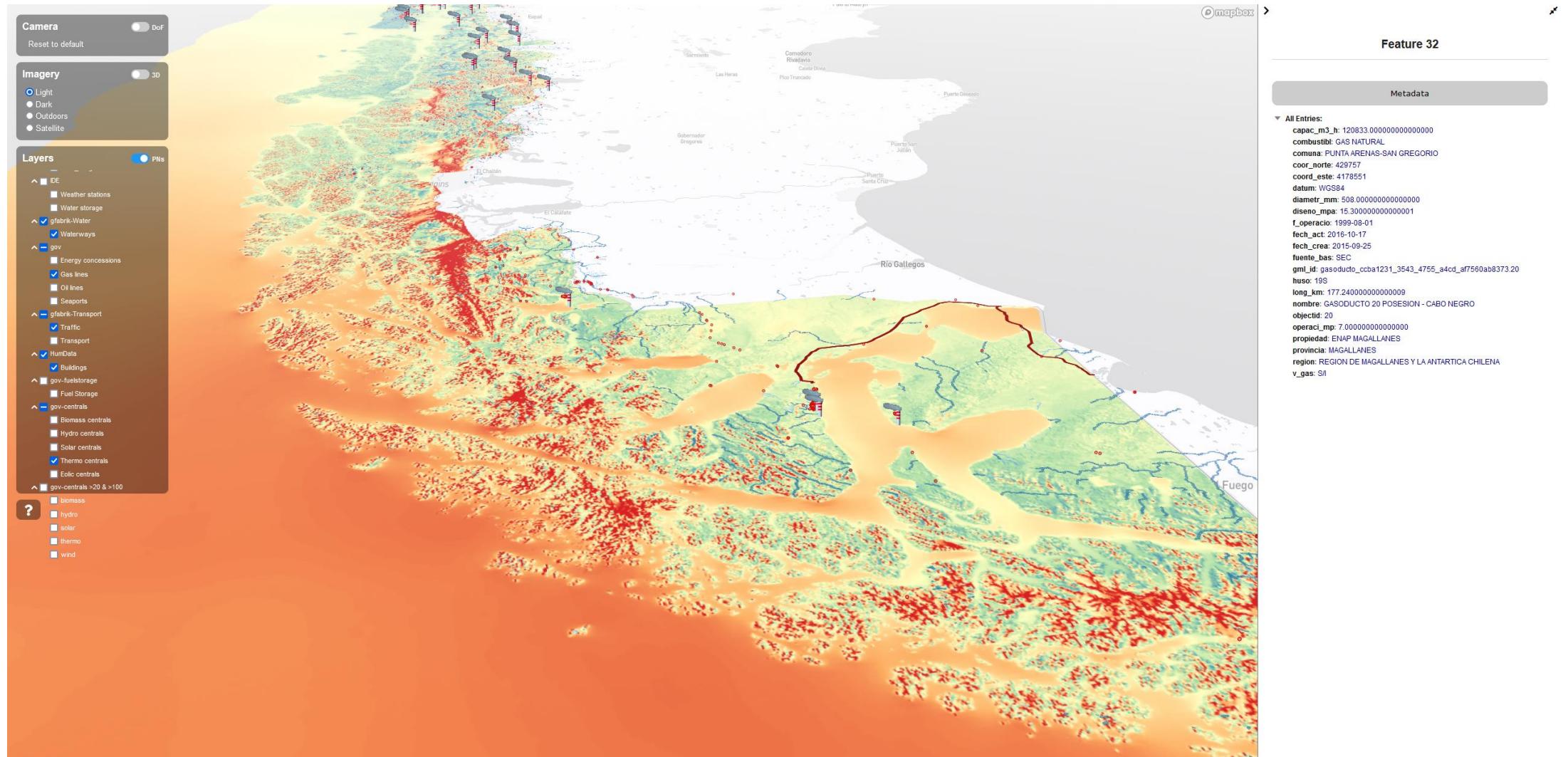


# Any Location

# The World Avatar (TWA)

## Representation of cross-domain data in Chile

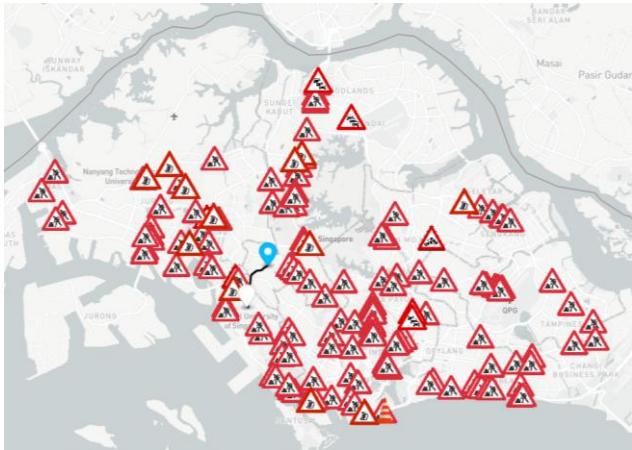
Scale - Country



# The World Avatar (TWA)

## Applicable and extendable to any location

Singapore



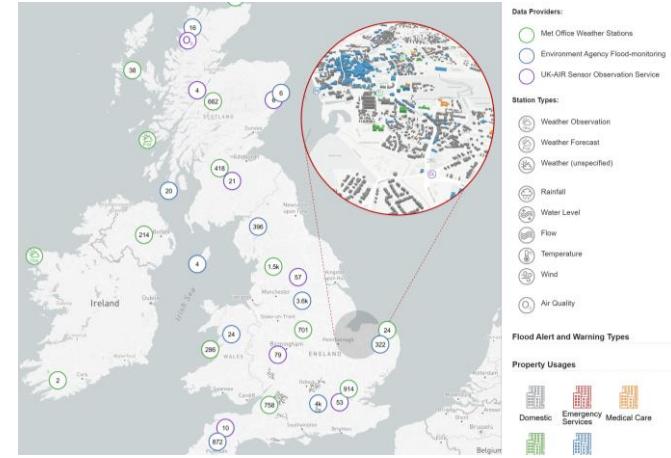
Germany



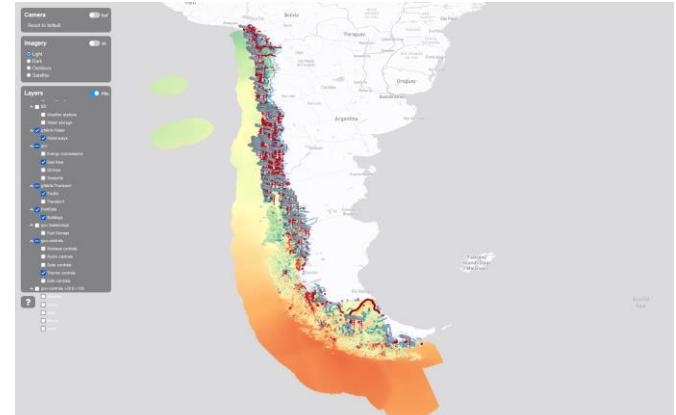
## The World Avatar

Any Location

UK



Chile

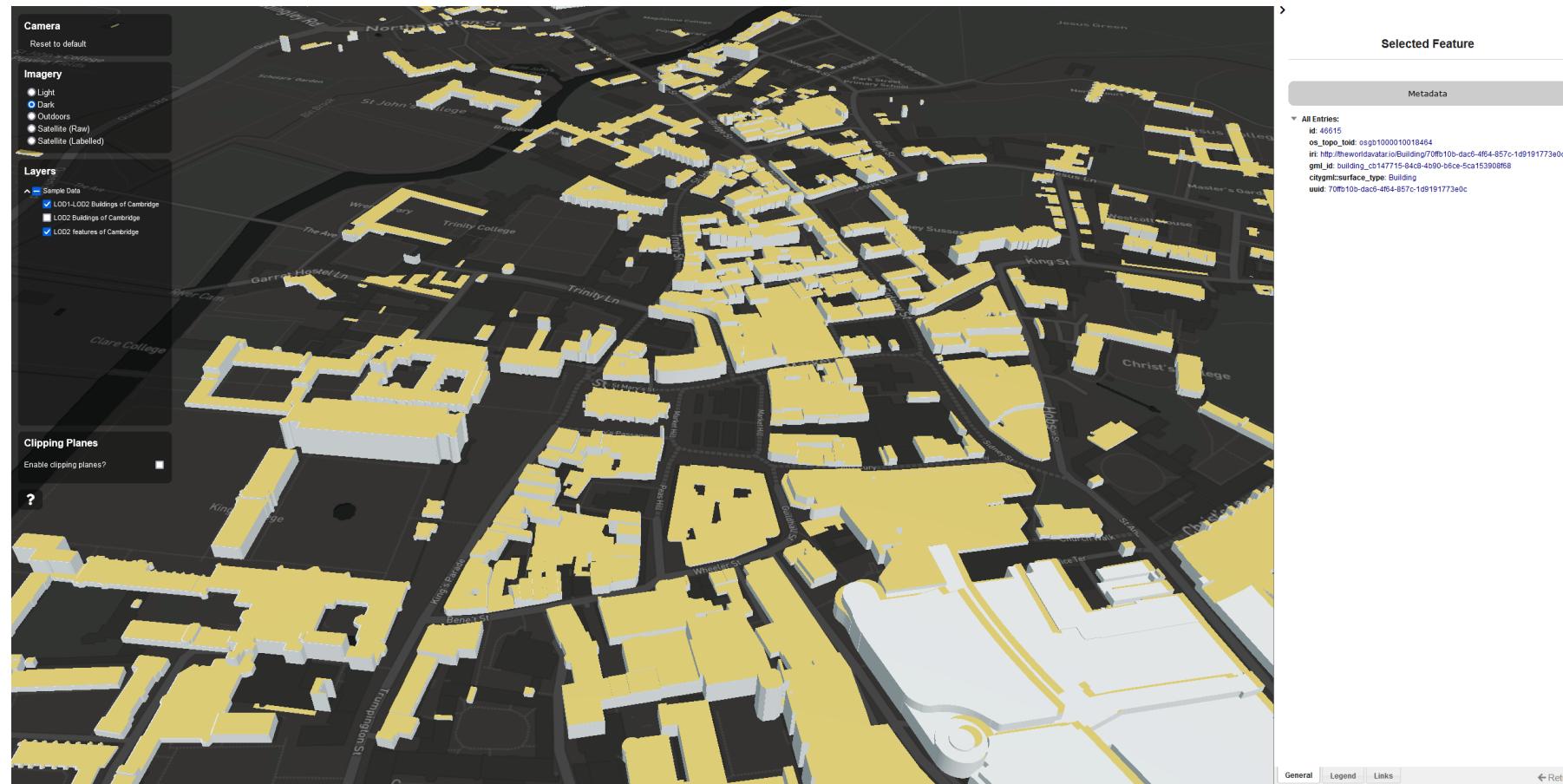


# Interfaces

# The World Avatar (TWA)

Representation of building data: Cambridgeshire

## Unified User Interfaces – 2D visualisation



# The World Avatar (TWA)

## BIM-GIS representation of Pirmasens: House 45

### Unified User Interfaces – 3D visualisation

**Smart City Pirmasens**

Pirmasens is an independent town in Rhineland-Palatinate, Germany, near the border with France. It was famous for the manufacturing of shoes, and has a population of 40,054 living within its land area of 61.37 sqkm.

The World Avatar, 2023

# The World Avatar (TWA) Unified User Interfaces

## Mobile App and Dashboard

