



CAMBRIDGE
CARES

CAMBRIDGE CENTRE
FOR ADVANCED RESEARCH AND
EDUCATION IN SINGAPORE LTD.



Prof Markus Kraft

CARES Director

Digital Transformation

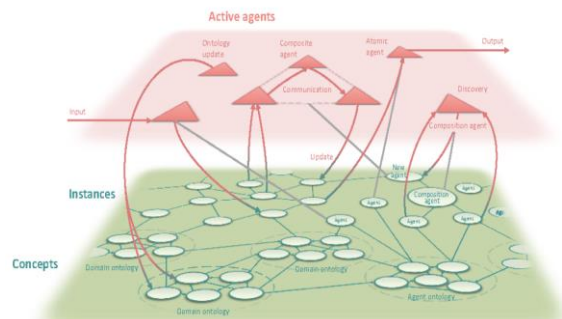
Ten Years of Digital Transformation at CARES

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



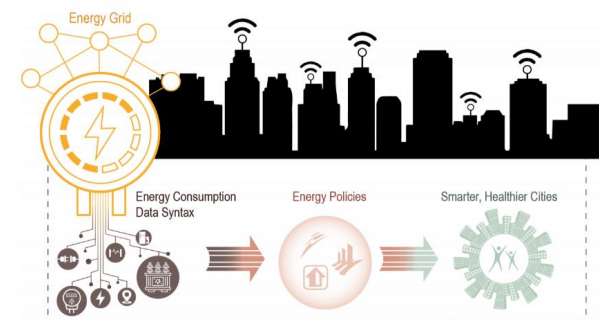
Cooling Singapore, exploring heat effects of industry, buildings and transport in Singapore



eCO₂EP, developing ways of transforming CO₂ from industrial processes into useful compounds (*completed*)



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

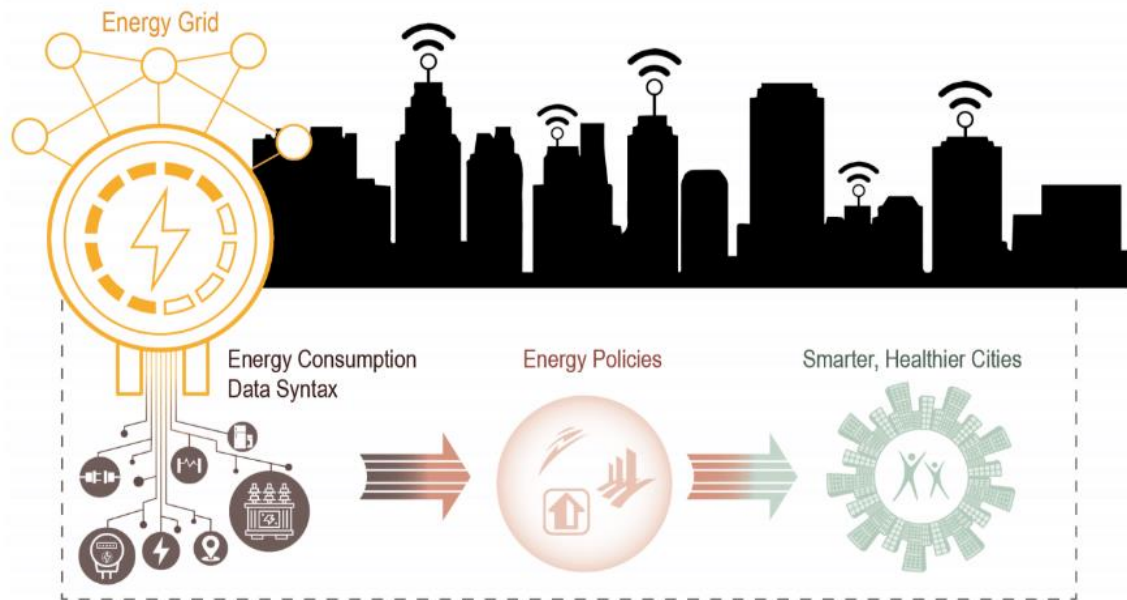


CEUS, Consumer Energy Usage Data in Smart City Development (*completed*)

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

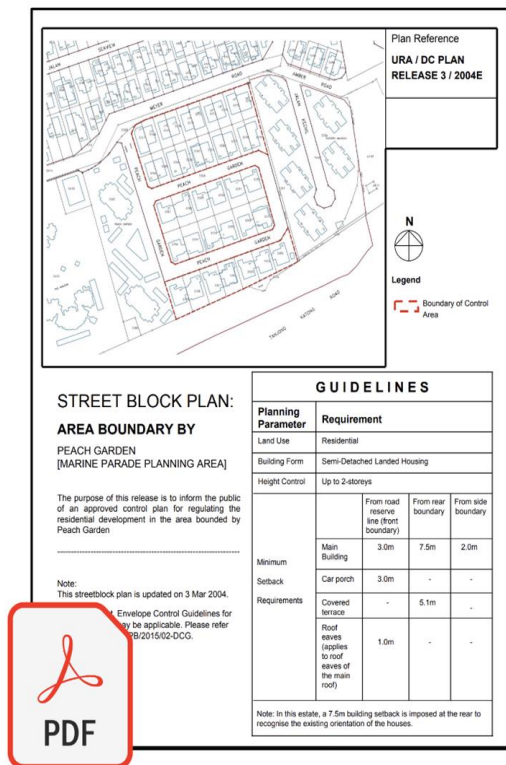
- Consumers could enjoy lower utility bills, select suitable retail electricity offerings, and harness renewable energy
- Building level energy consumption and costs could reduce
- Enhance grid resilience

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.

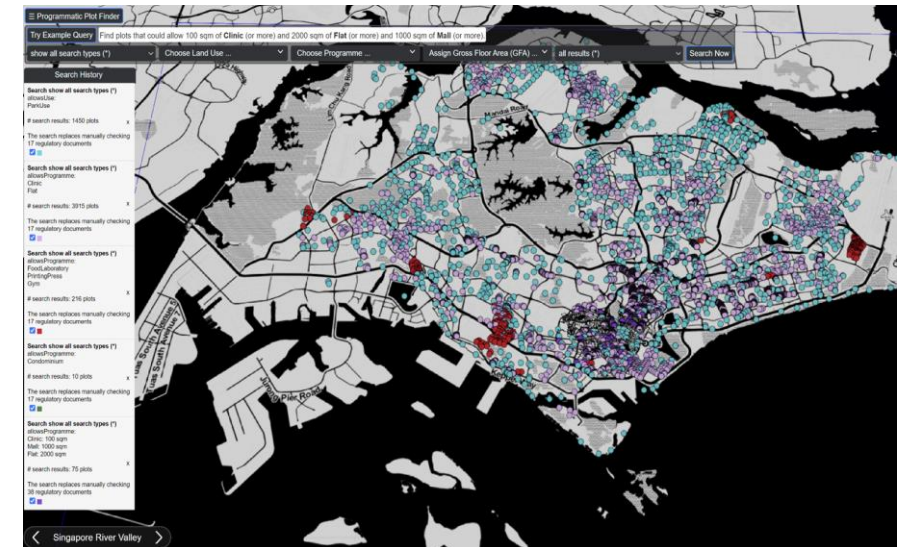
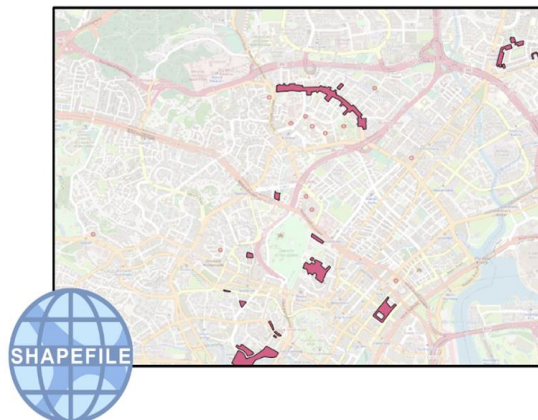
PDF documents



Online text and iconography



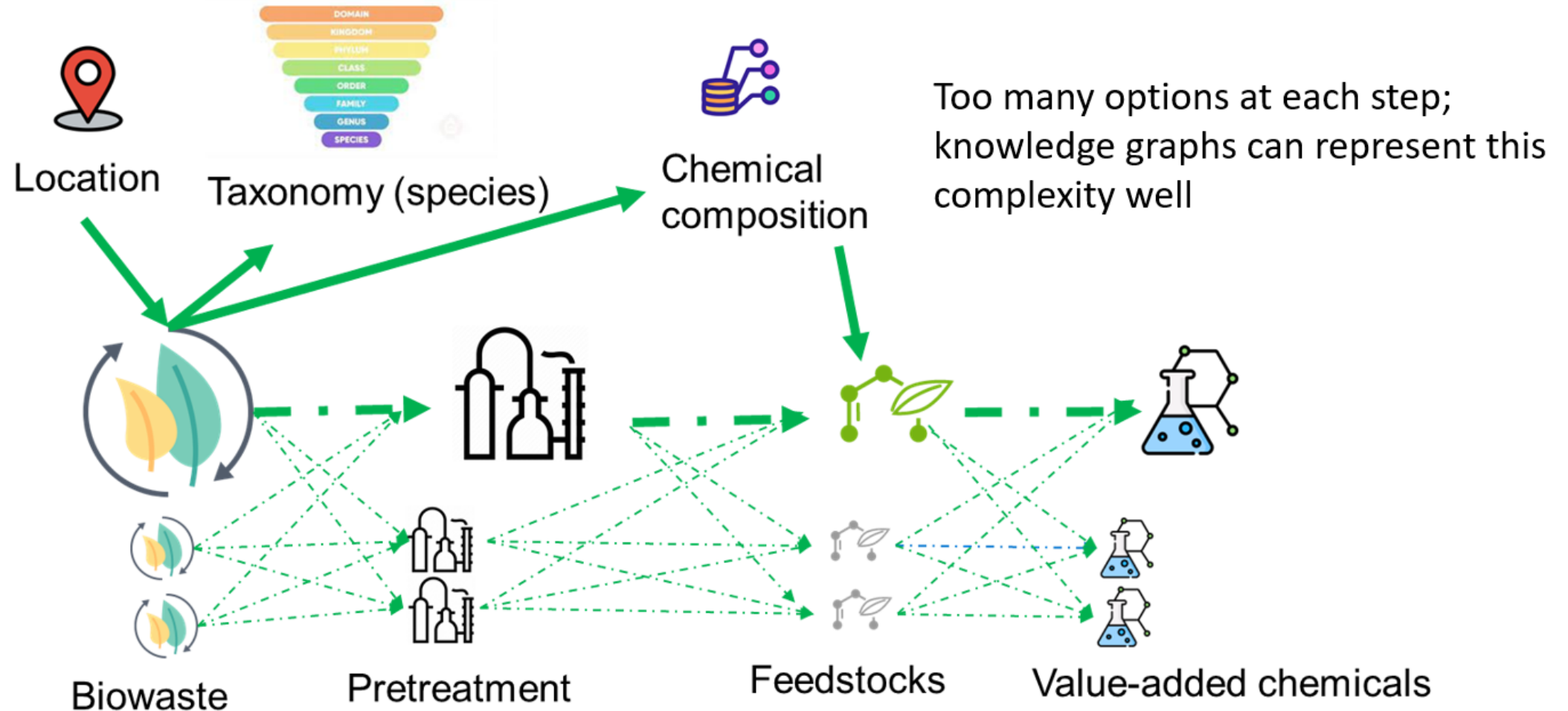
GIS layer (data.gov.sg)



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**?

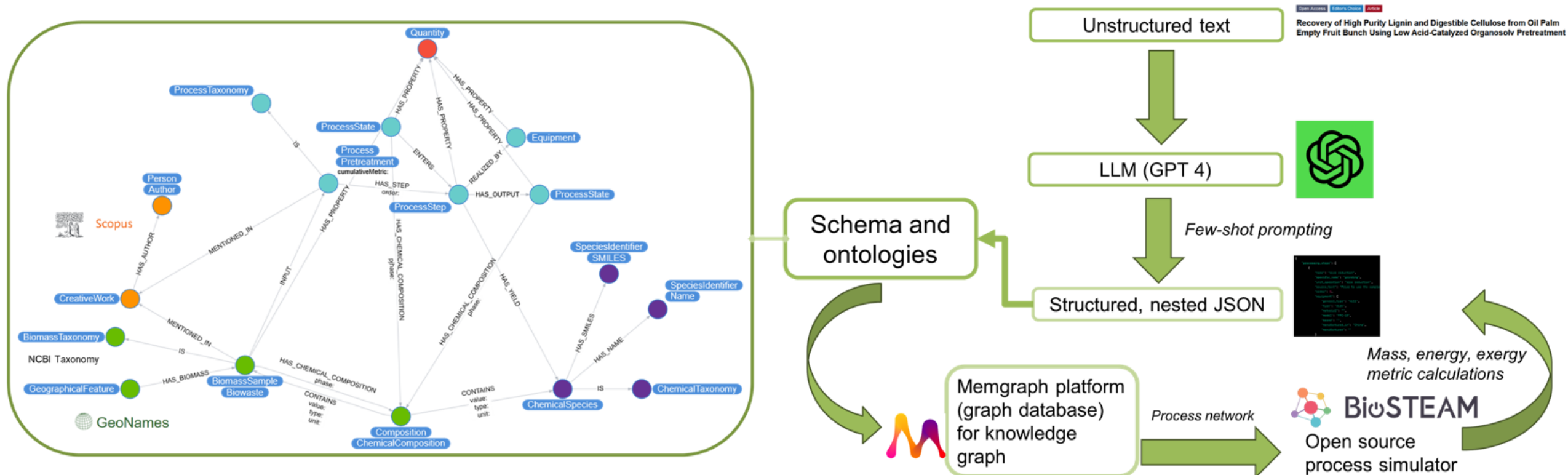


Ten Years of Digital Transformation at CARES

Knowledge graphs for the biowaste-to-chemicals domain

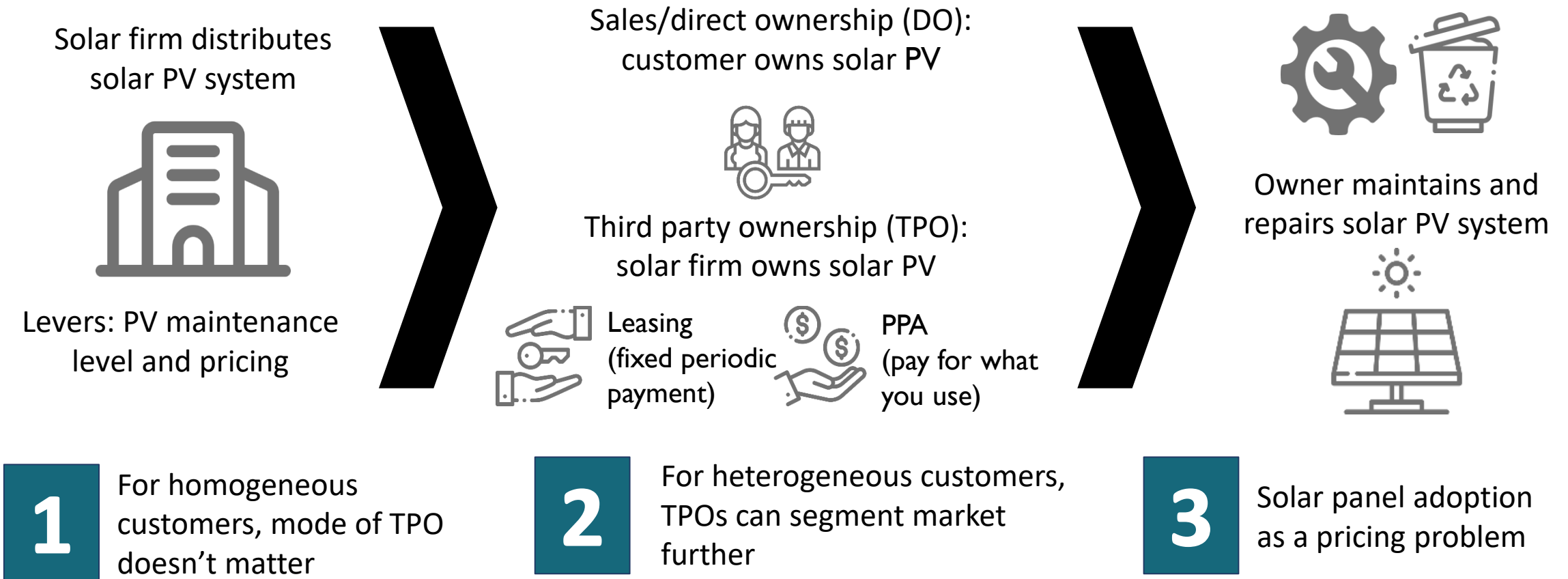
What are the **most sustainable routes** from **biowaste** to **value added chemicals** and **how can we find them**?

Workflow for knowledge graph population



Ten Years of Digital Transformation at CARES

Incentivizing Solar Panel Adoption

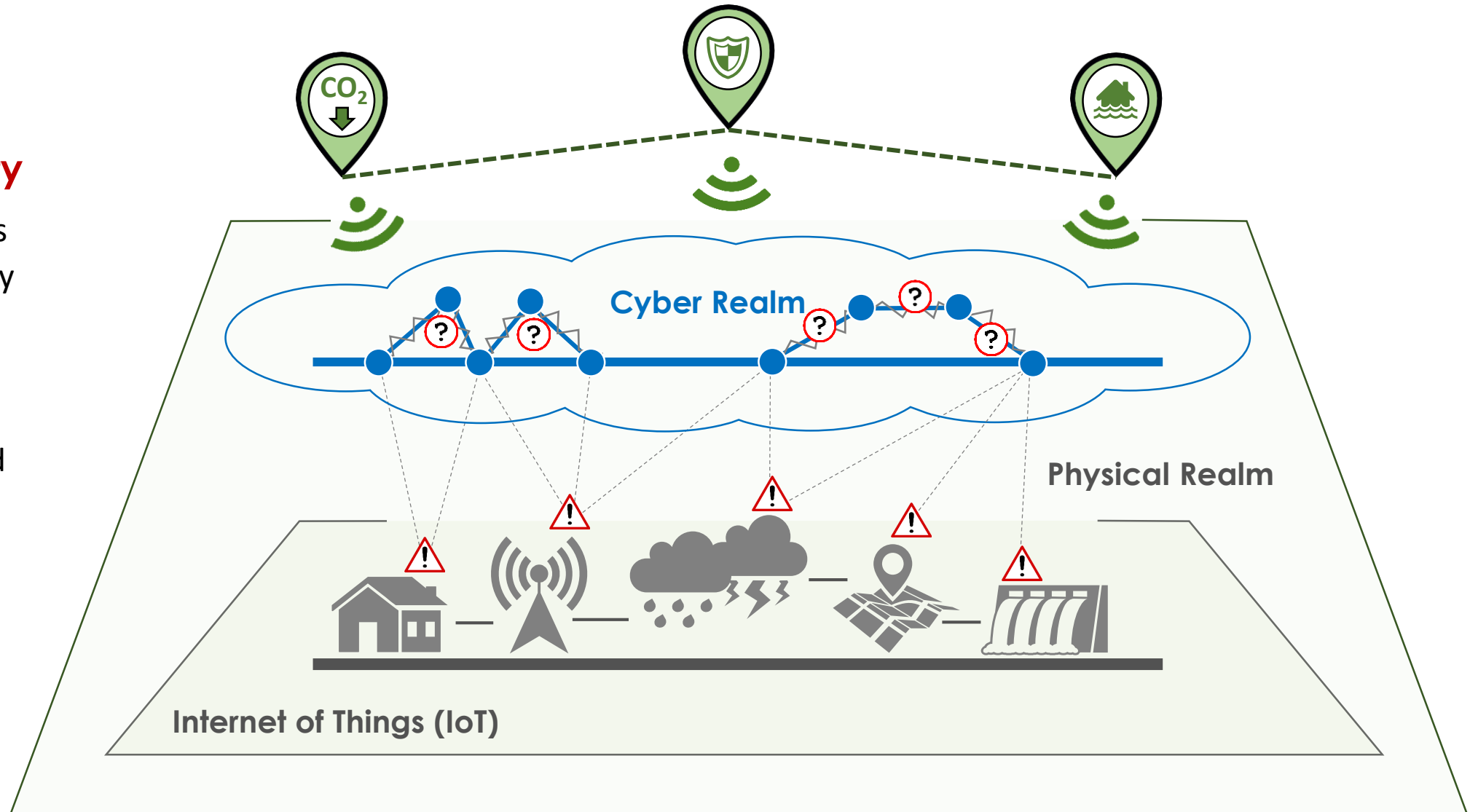


Building on product-as-service models for clean technologies, we **can leverage data-driven approaches** to generate **further market insights**

The Problem

Low Interoperability

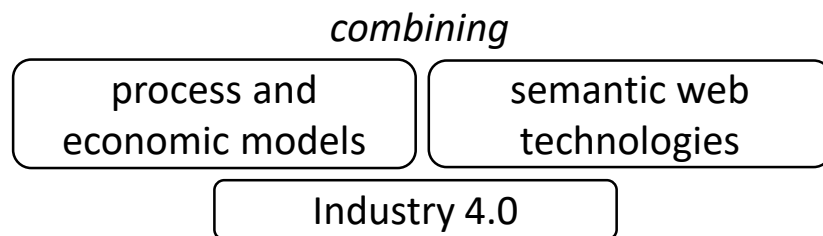
- Different protocols and data ambiguity
- High friction in exchange and integration
- Lock-in effects and surging switching cost



Ten Years of Digital Transformation at CARES

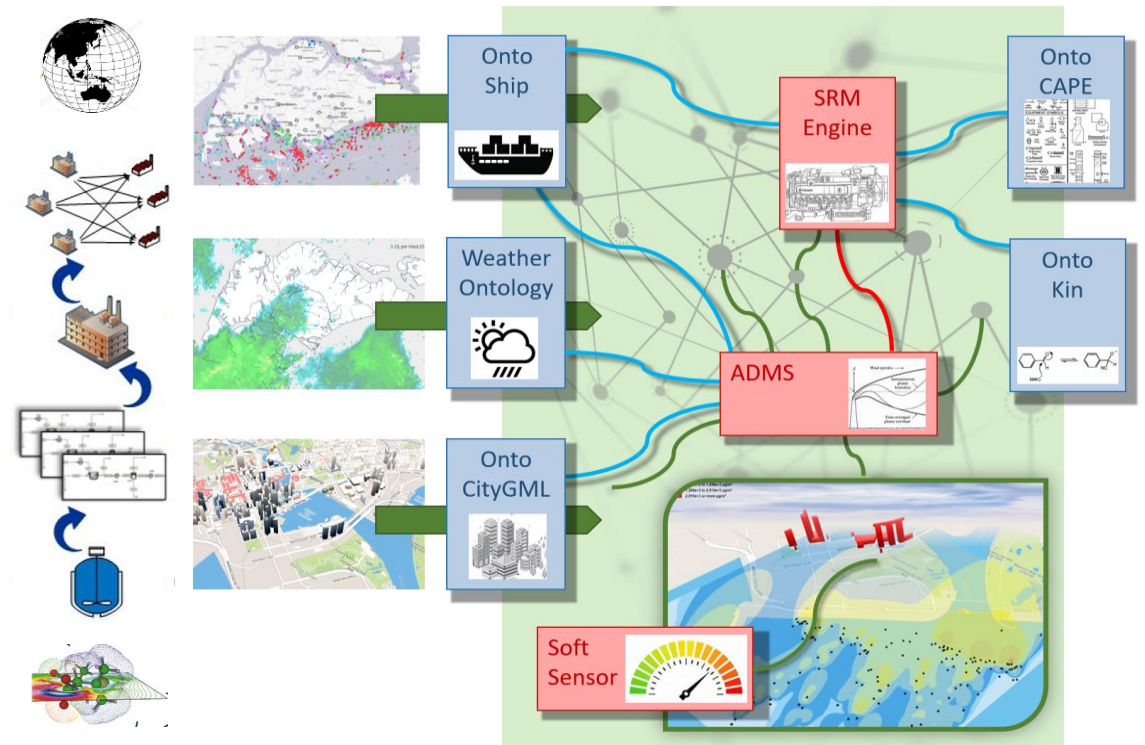
J-Park Simulator (JPS) – an interdisciplinary research programme within C4T

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



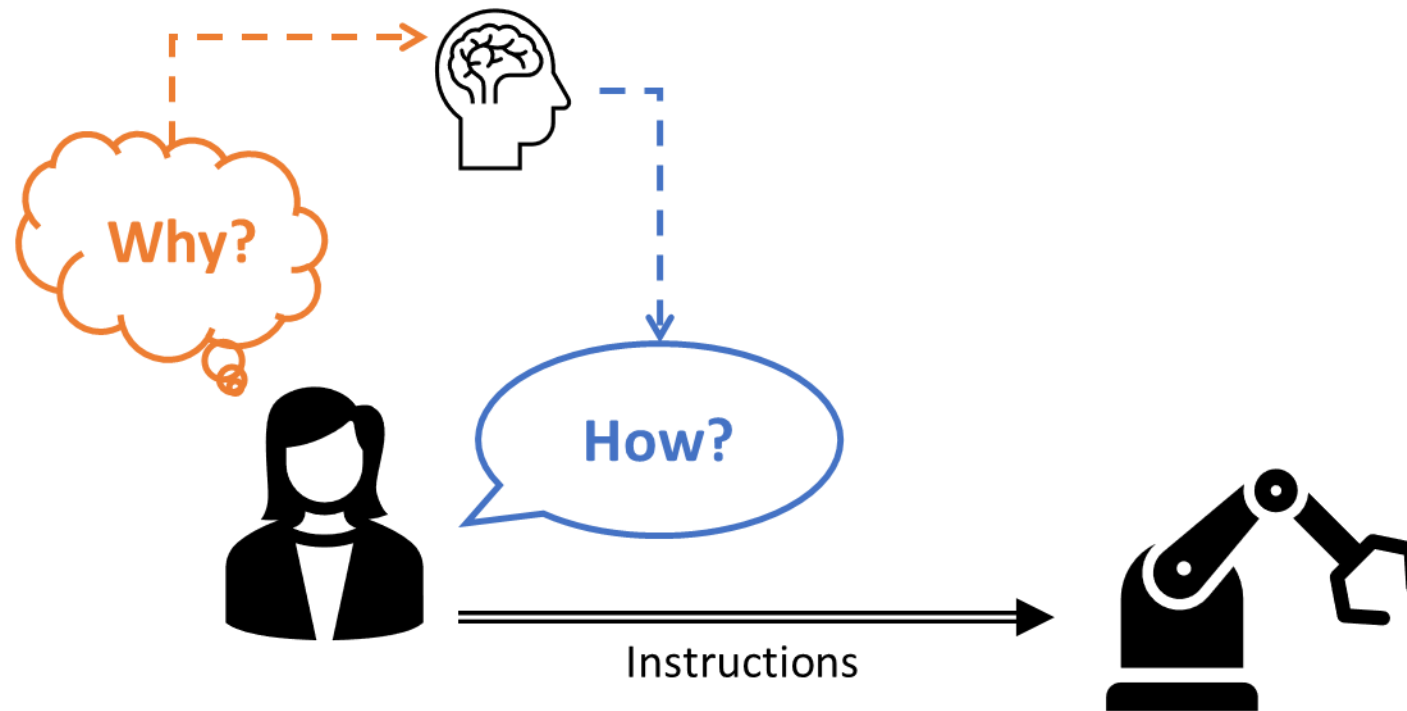
JPS sets the benchmark for The World Avatar

- JPS successfully estimated the total yearly emissions from Jurong Island (29MTCO₂) 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.

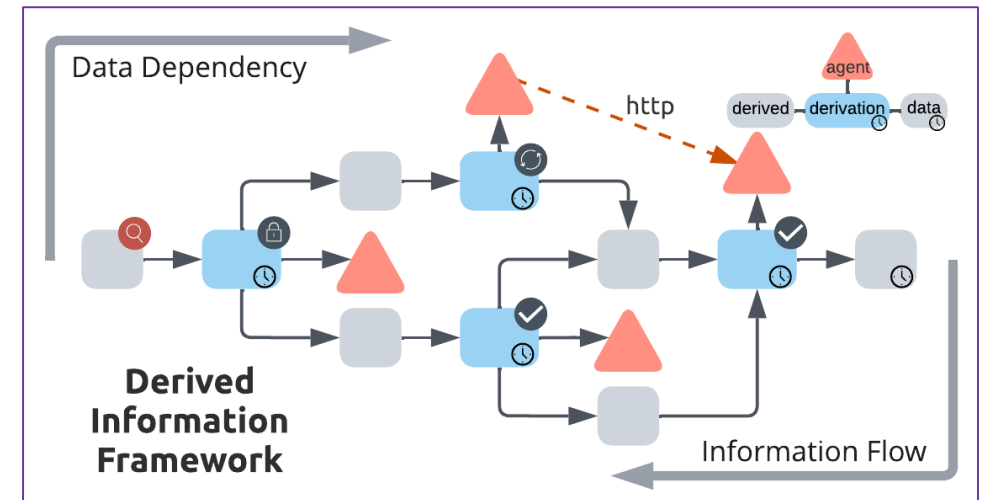
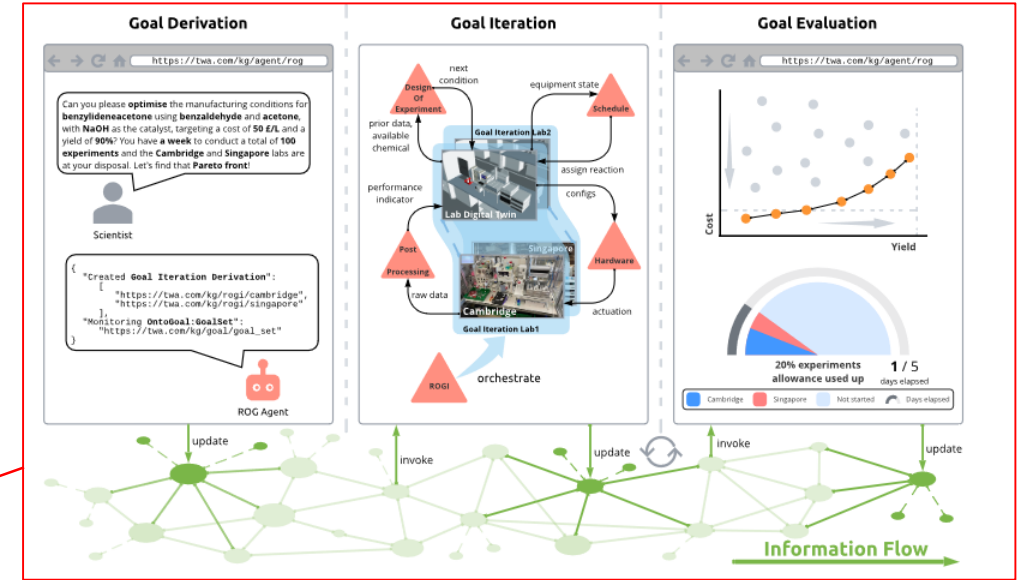
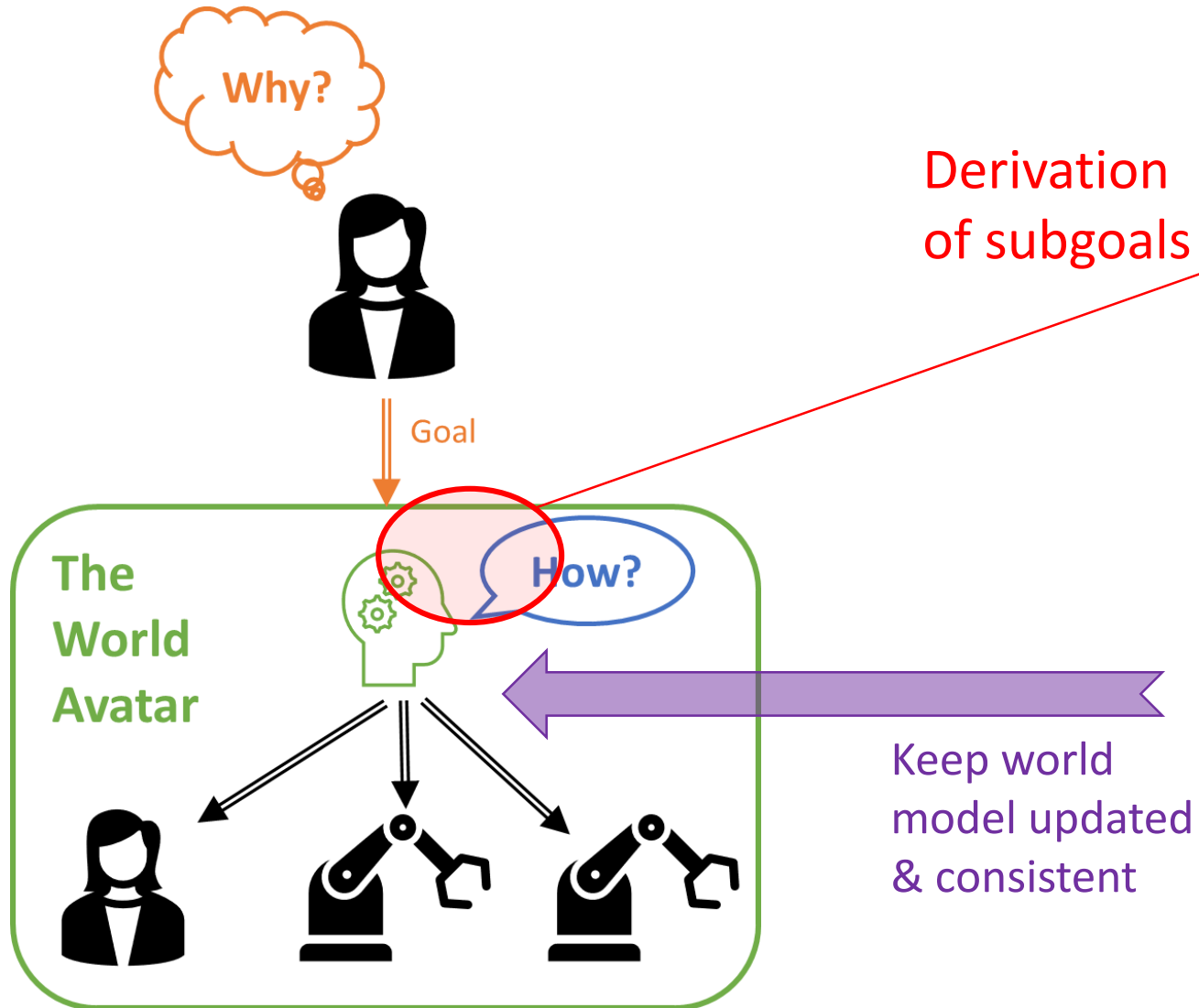


A change in
perspective

Human-in-the-loop – so far...



Human-in-the-loop - TWA

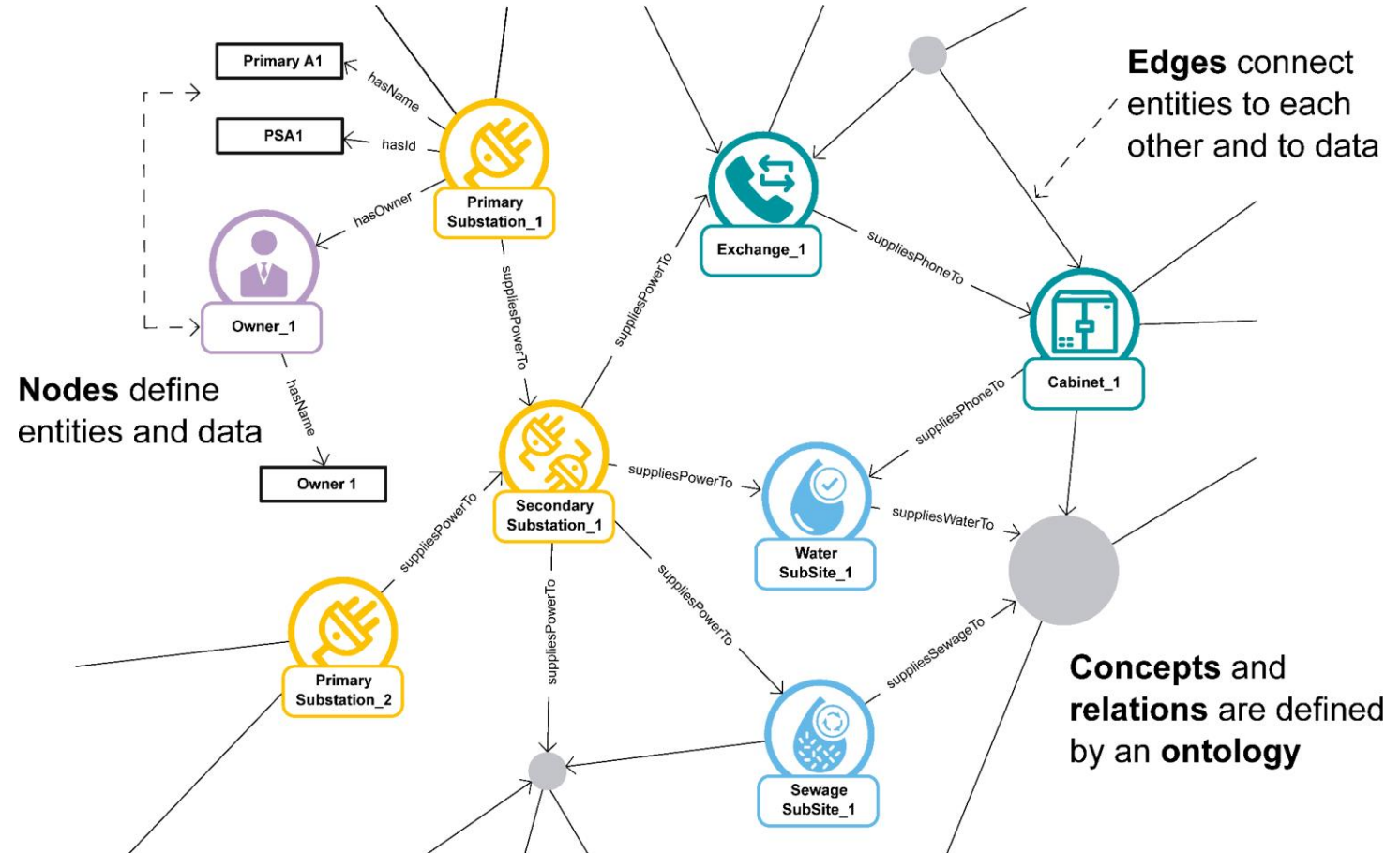


The Proposed Solution

- **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



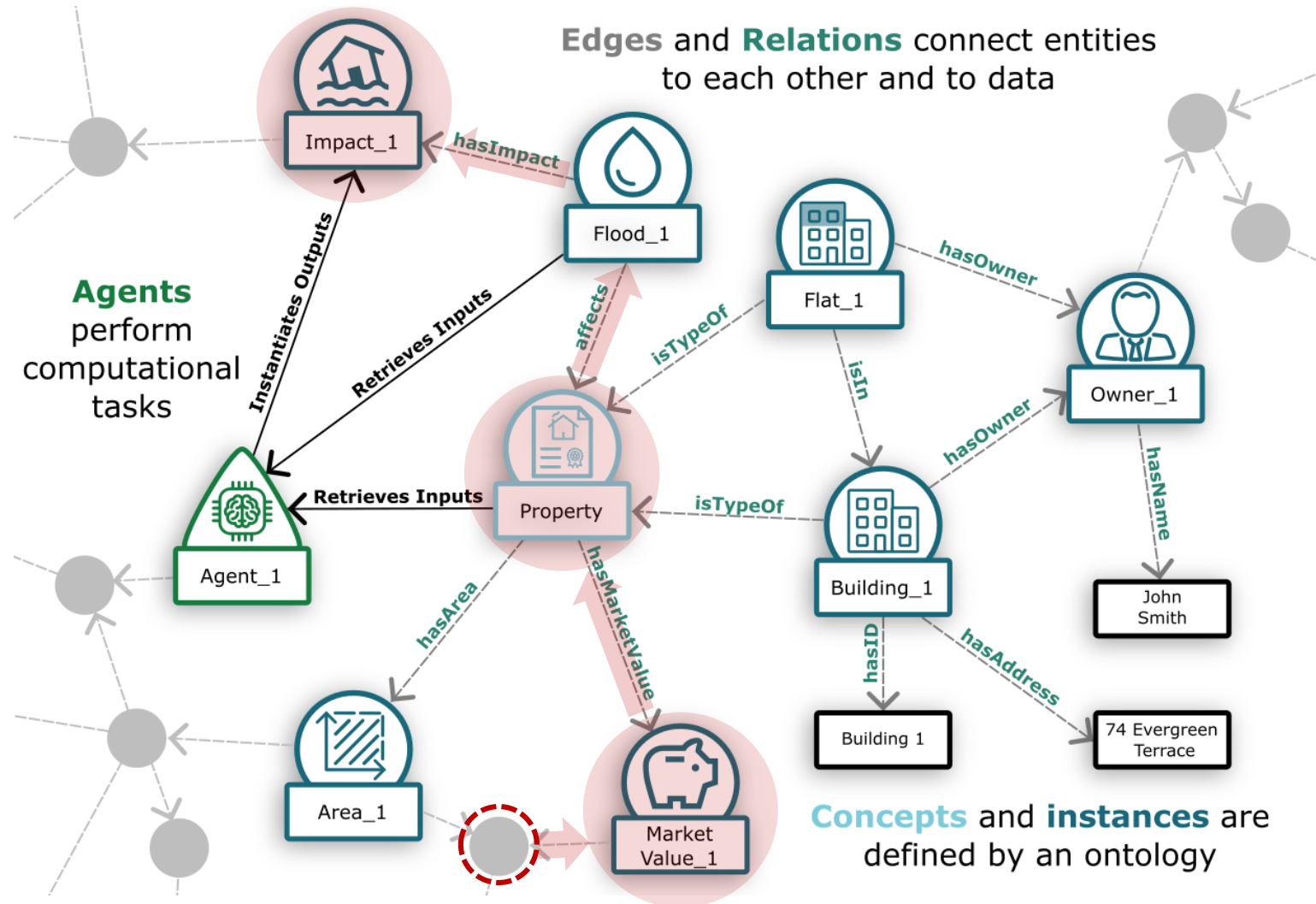
SOURCE:
https://commons.wikimedia.org/wiki/File:FAIR_data_principles.jpg



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

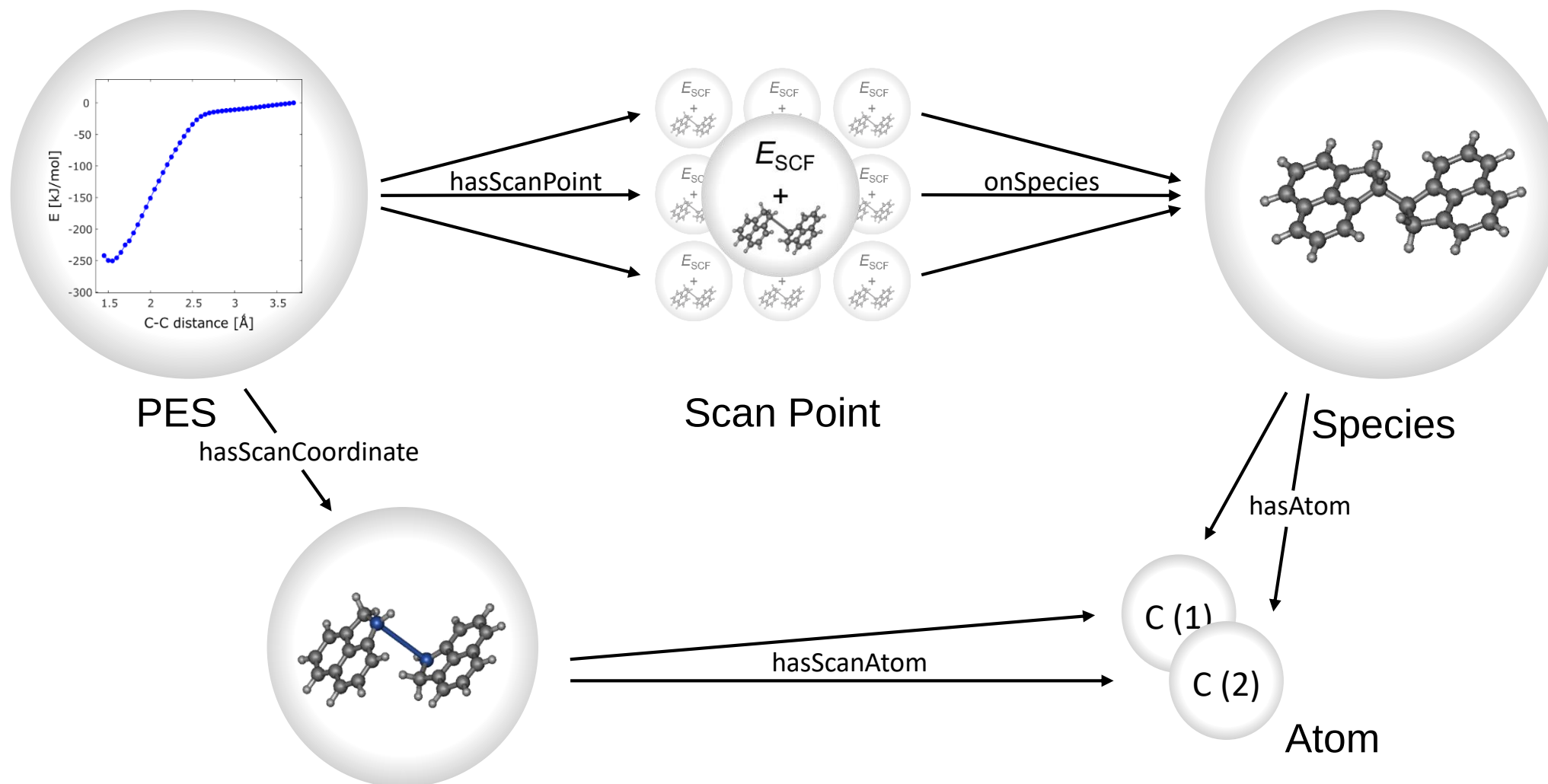
Explore parallel-world scenarios to safely predict and explore the real-world impacts of changes and decisions

Any Scale

The World Avatar (TWA)

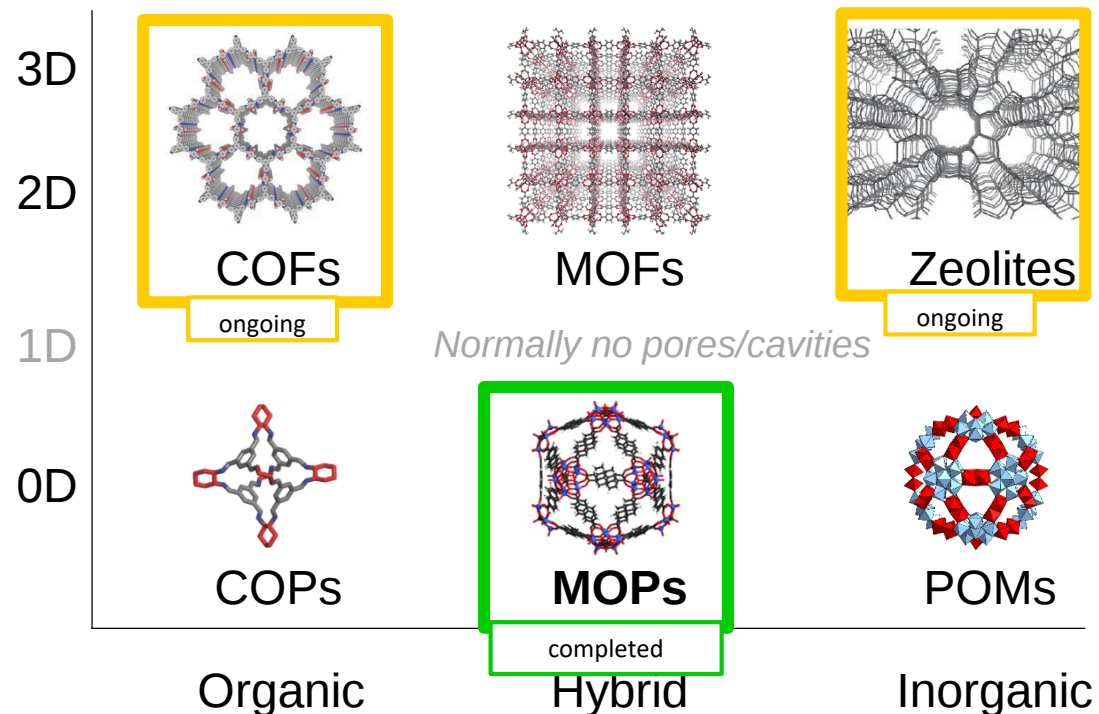
Automated atomistic understanding

Scale - Molecular



The World Avatar (TWA)

Automated derivation of high value materials



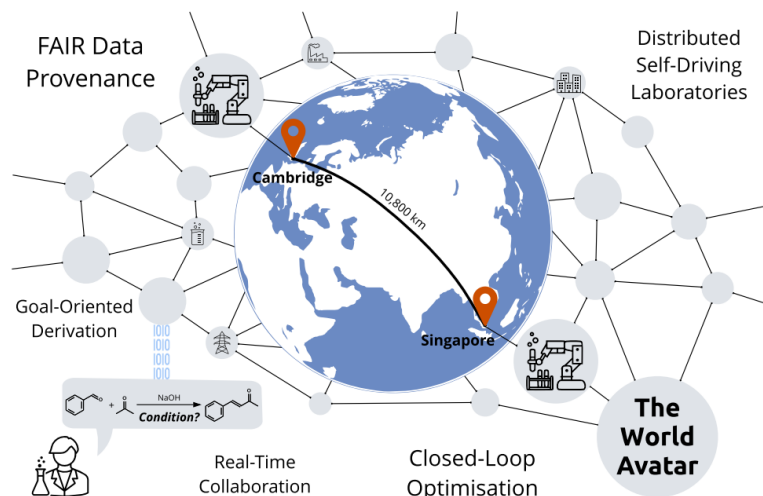
- Materials are made of chemical building units (CBUs).
- By changing CBUs, one can rationally design and synthesize a plethora of new materials with tailoring porosity/cavity sizes, electronic structure and chemical properties.

The World Avatar (TWA)

Efficient Automation Processes

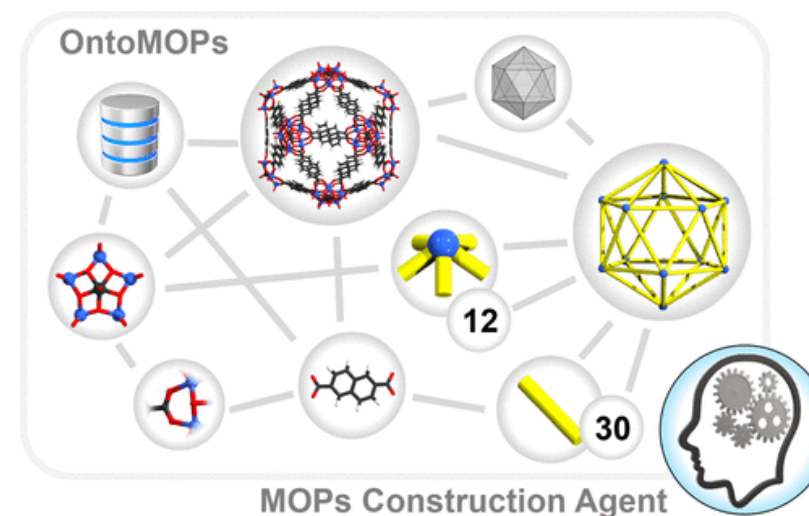
Scale - Molecular

Chemical synthesis optimisation



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

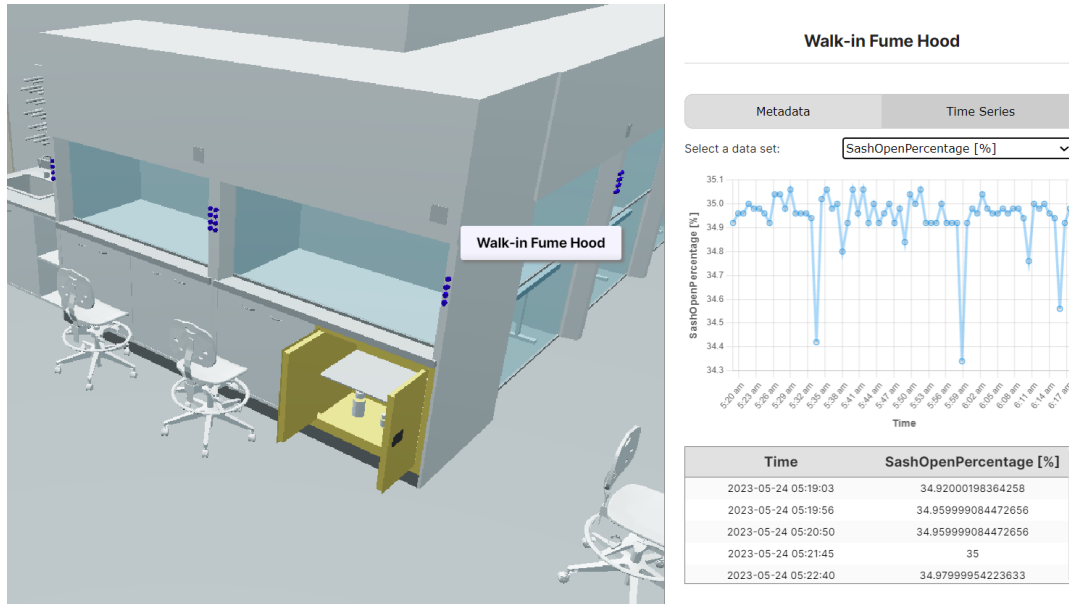
Chemical molecular design



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

Scale - Building



Is fume hood sash open?
Is fume hood currently unused?

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

[KG EmailAgent] - Fumehoods and WalkIn-Fumehoods Sash and Occupancy Alert! 🔍

astoria-cares@outlook.com
To: wilson1010x@gmail.com, Wilson Ang

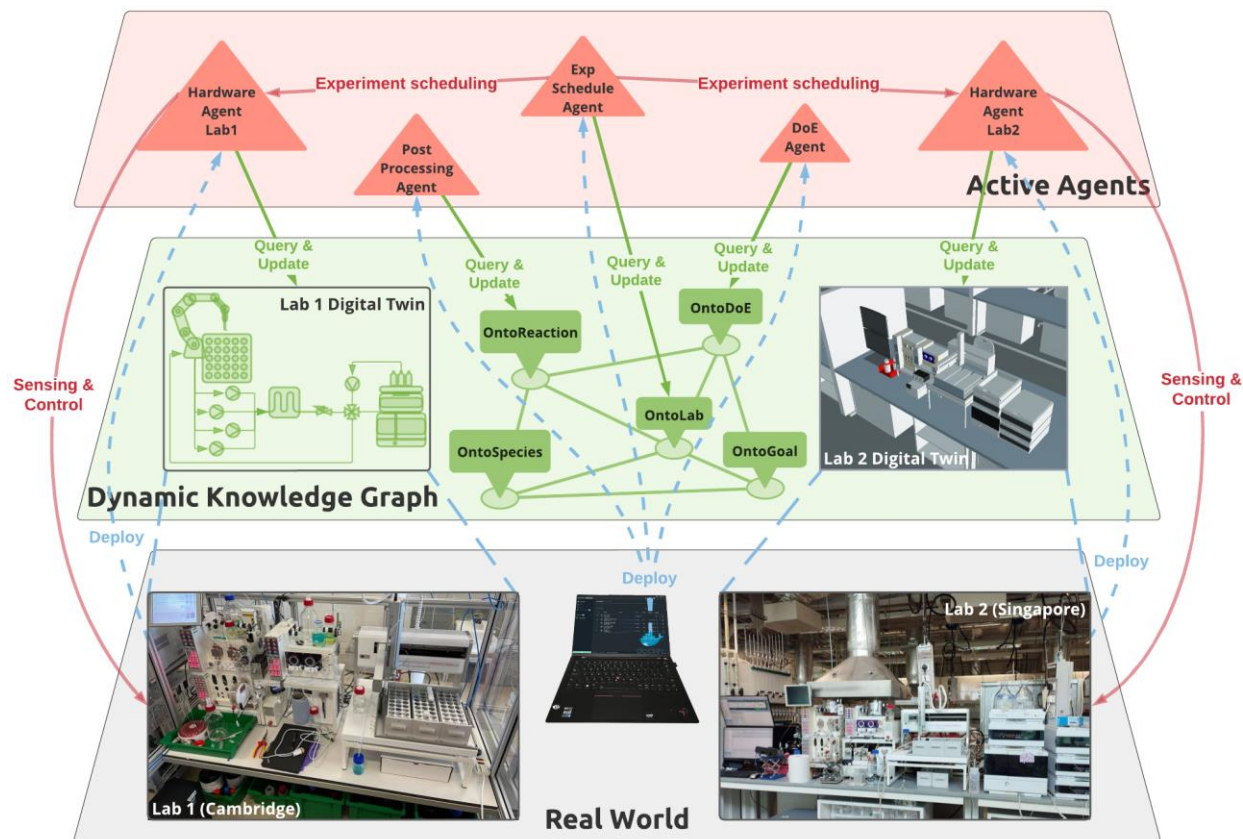
What follows is an automated email generated by the EmailAgent agent on behalf of another KG service.
Please do not reply.

The following devices (FH-02, FH-08) are unoccupied and have a sash opening above the threshold of 50.0%. Please close the sash for these fumehoods and walkin-fumehoods if they are unoccupied and not in use. Listed below are the fumehoods, walkin-fumehoods, their occupied state and sash opening values:

Devices	Occupied State	Sash Opening
FH-01	This device does not have an occupied state.	30.40 % since the following timestamp: 2023-05-03 06:18:50 AM UTC
FH-02	Not occupied since the following timestamp: 2023-04-11 04:27:16 AM UTC	90.60 % since the following timestamp: 2023-05-03 06:18:50 AM UTC
FH-03	This device does not have an occupied state.	30.66 % since the following timestamp: 2023-05-03 06:18:50 AM UTC
FH-04	This device does not have an occupied state.	71.74 % since the following timestamp: 2023-05-03 06:18:50 AM UTC
FH-05	This device does not have an occupied state.	18.50 % since the following timestamp: 2023-05-03 06:18:50 AM UTC
FH-06	This device does not have an occupied state.	18.58 % since the following timestamp: 2023-05-03 06:18:50 AM UTC
FH-07	This device does not have an occupied state.	28.94 % since the following timestamp: 2023-05-03 06:18:50 AM UTC
FH-08	Not occupied since the following timestamp: 2023-04-19 01:58:19 AM UTC	103.24 % since the following timestamp: 2023-05-03 06:18:50 AM UTC

The World Avatar (TWA) Augmented CARES Lab

Scale - Building



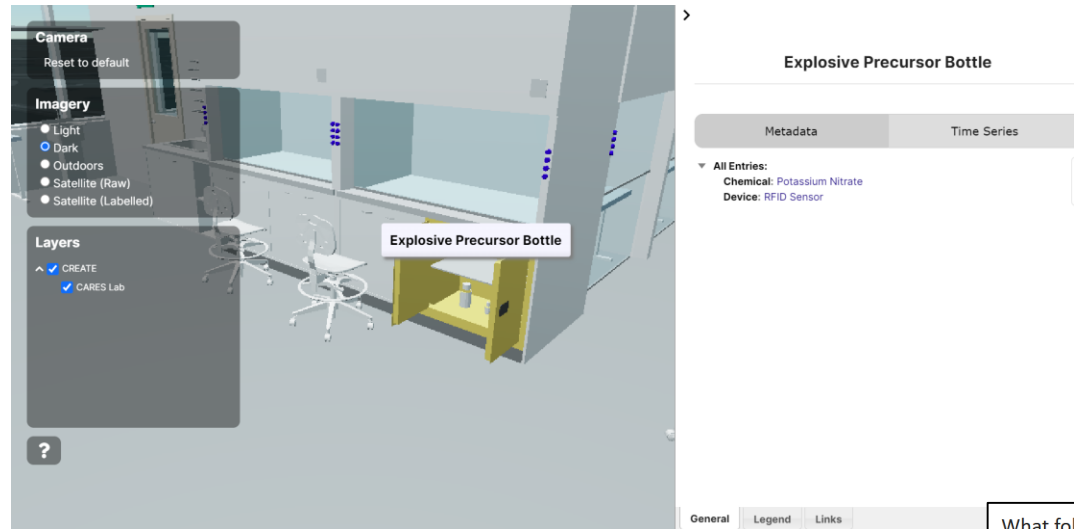
Experiments

- 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

Scale - Building



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: 0000000000000A000009727 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: c0ccfd8a329

Local IP Address: 172.23.0.2

The World Avatar (TWA)

Scale - Building

BIM-GIS representation of Pirmasens: House 45

Camera

Imagery

Layers

- ☒ Augmented Pirmasens
- ☒ City
- ☒ House 45

Clipping Planes

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

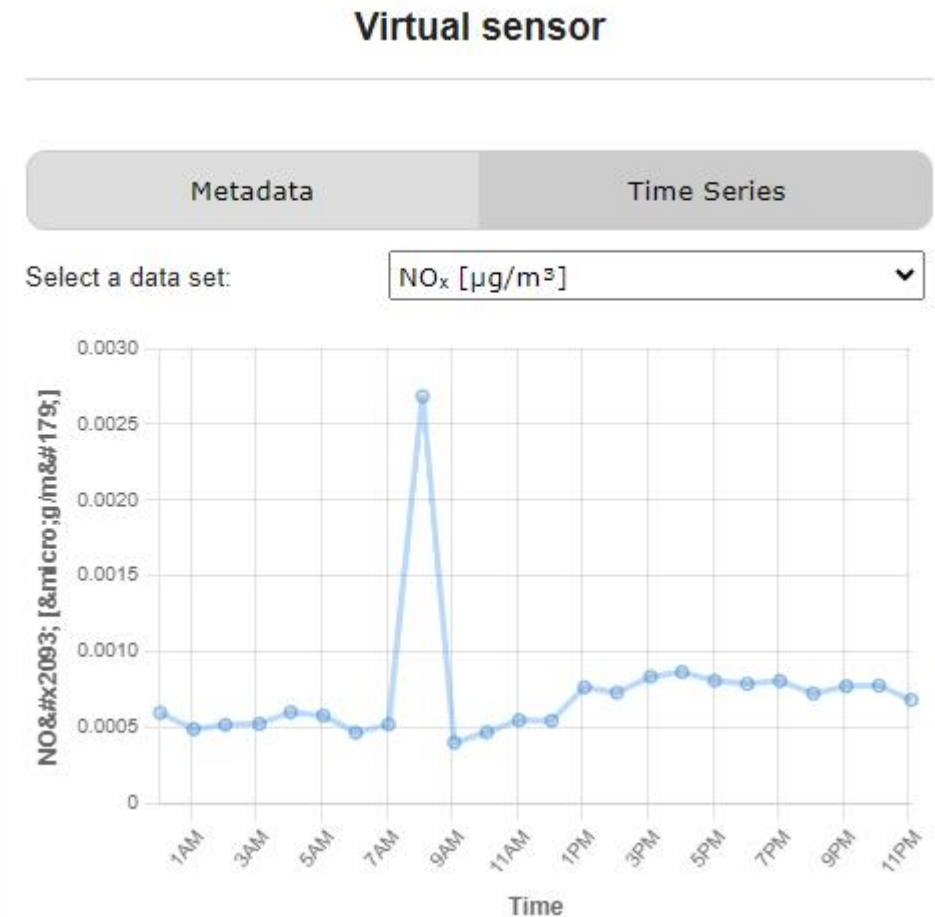
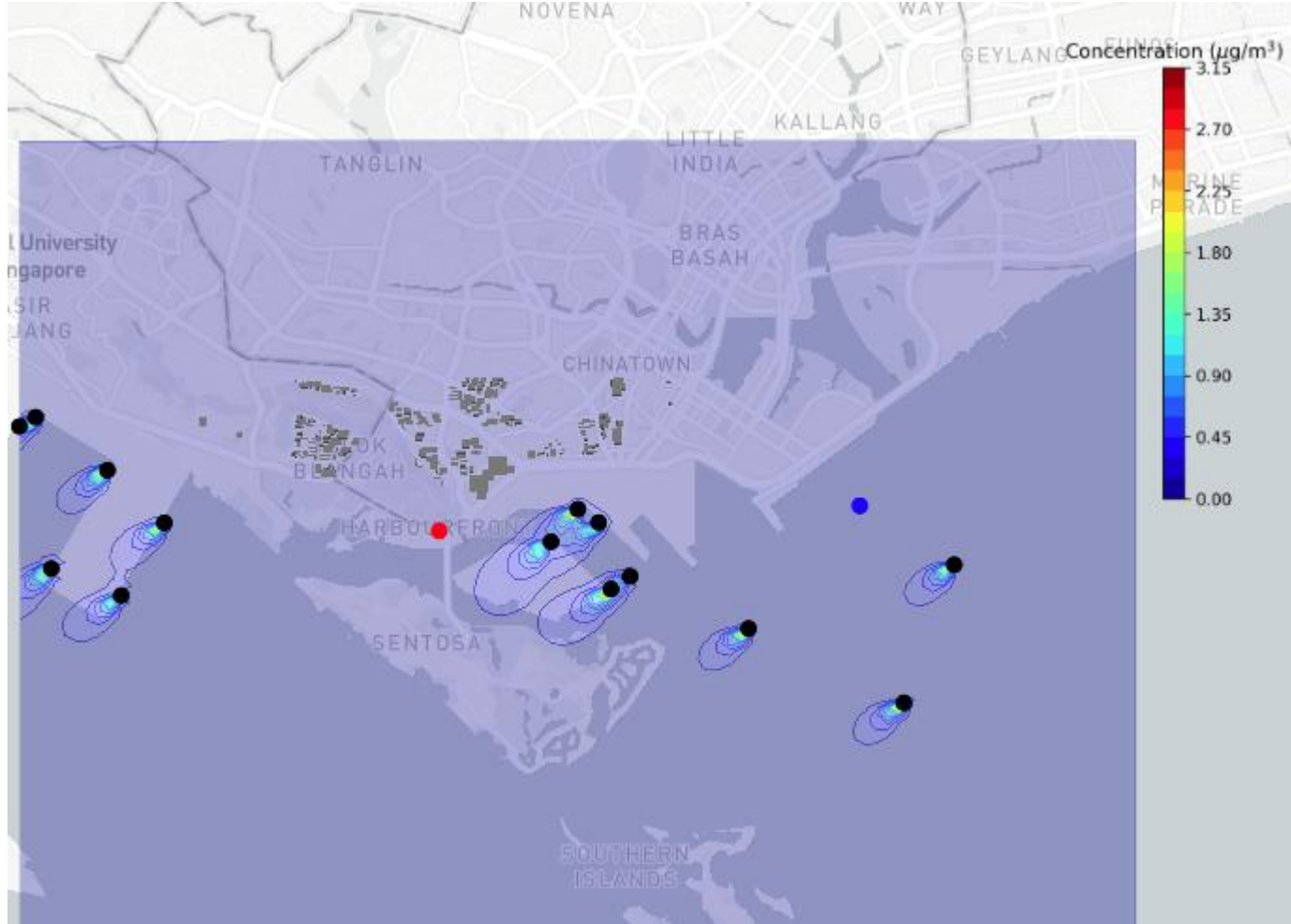
- Type:** Monocrystalline
- Performance:** 415 - 430 Wp
- Panel efficiency:** 21.25 ~ 22.02%
- Cost per module:** 154€
- Vendor:** Axitec Energy
- Dimensions (L x W x H):** 1722 × 1134 × 30 mm
- Weight:** 21.8kg

General | **Legend** | **Links** | [Return](#)

The World Avatar (TWA)

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

Scale - City



The World Avatar (TWA)

Scale - City

Augmenting simulation data with sensor data

- Representation of ambient environmental variables (Noise, Light, Speed) timestamped with coordinates and collected using existing mobile phone sensors, overlaid 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 _x (ppb)	< 1 (Good)
O ₃ (ppb)	< 1 (Good)
SO ₂ (ppb)	< 1 (Good)
PM2.5 (µg/m³)	< 1 (Good)
PM10 (µg/m³)	< 1 (Good)



The World Avatar (TWA)

Augmenting simulation data with sensor data

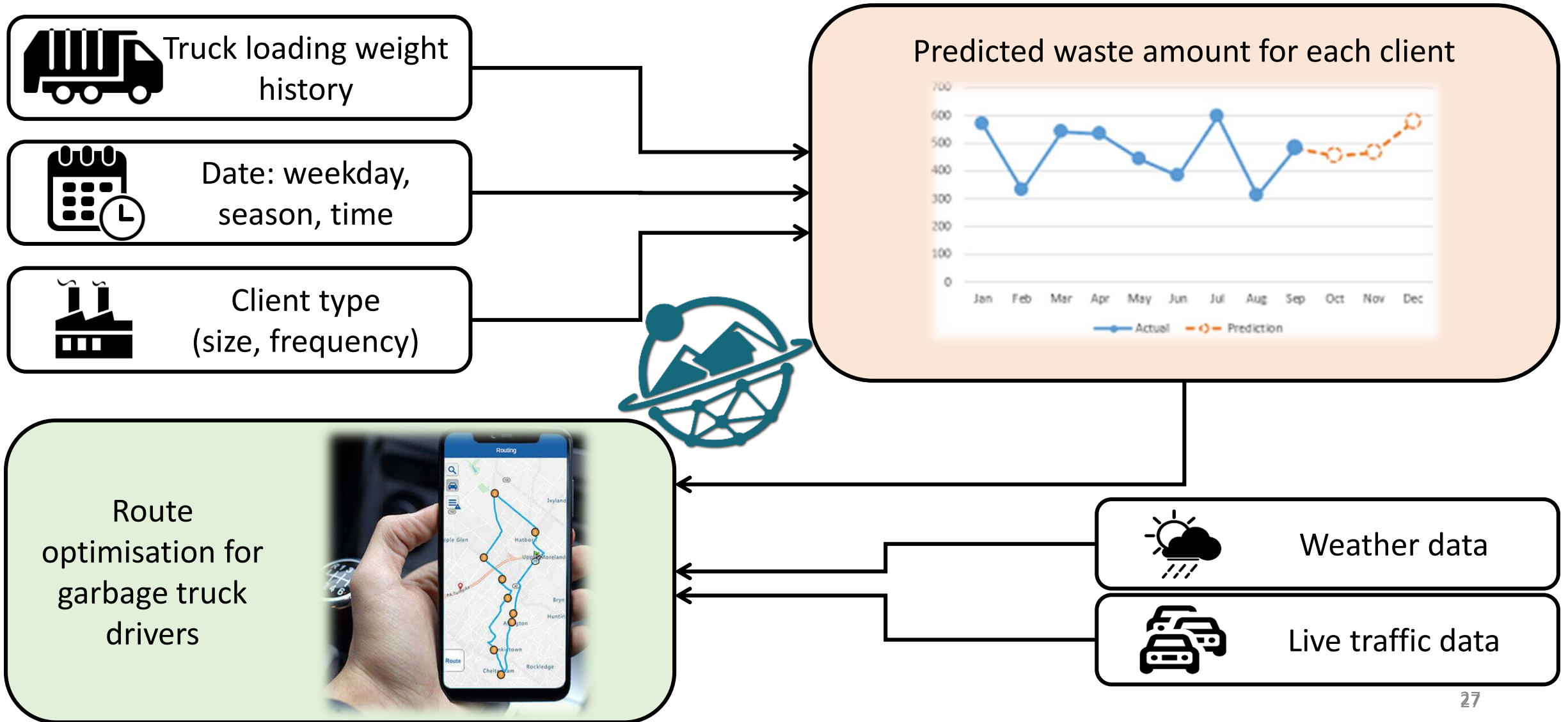
Scale - City

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 _x (ppb)	482 (Moderate)
O ₃ (ppb)	86 (Unhealthy)
SO ₂ (ppb)	84 (Moderate)
PM2.5 (µg/m³)	128 (Unhealthy)
PM10 (µg/m³)	247 (Unhealthy)



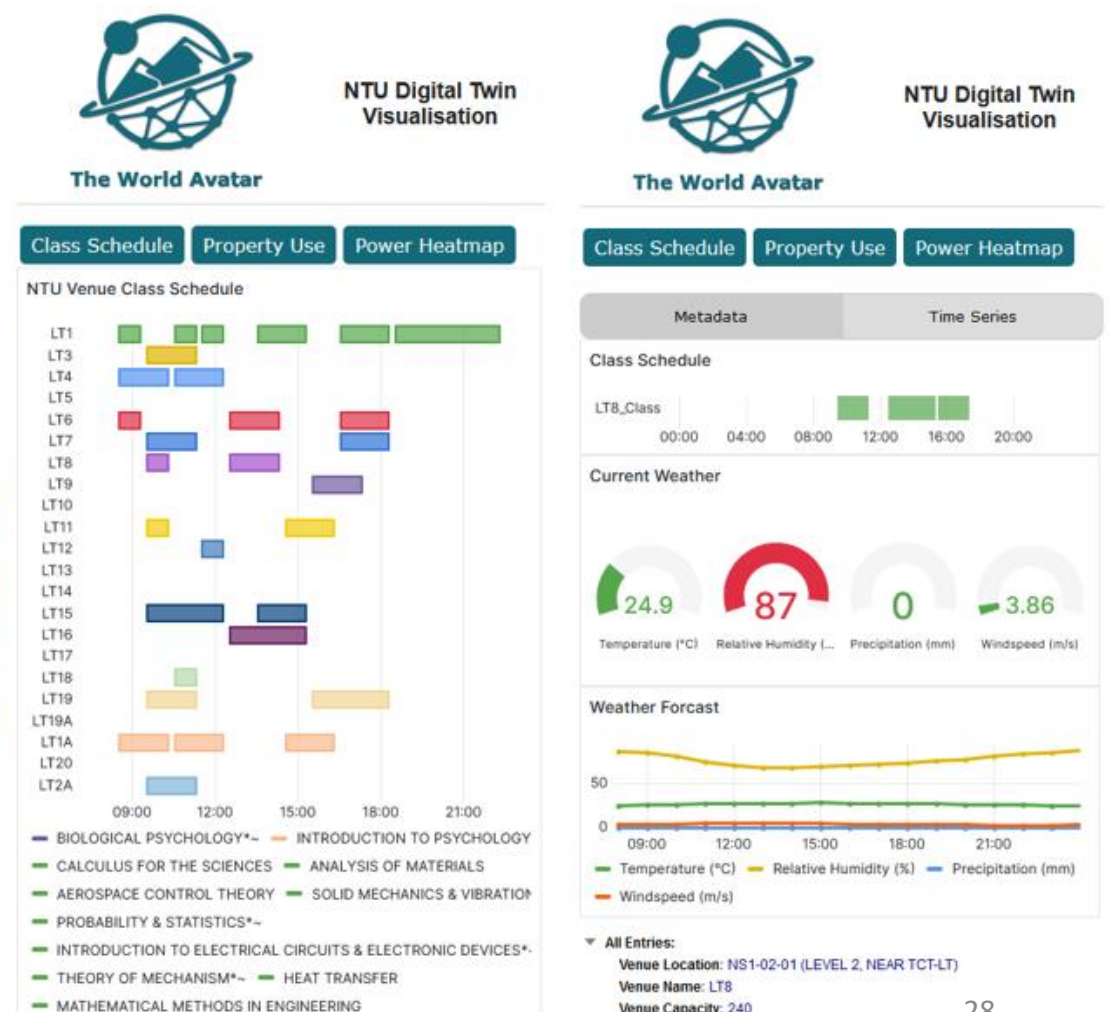
The World Avatar (TWA)

Route optimisation for waste collection



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.

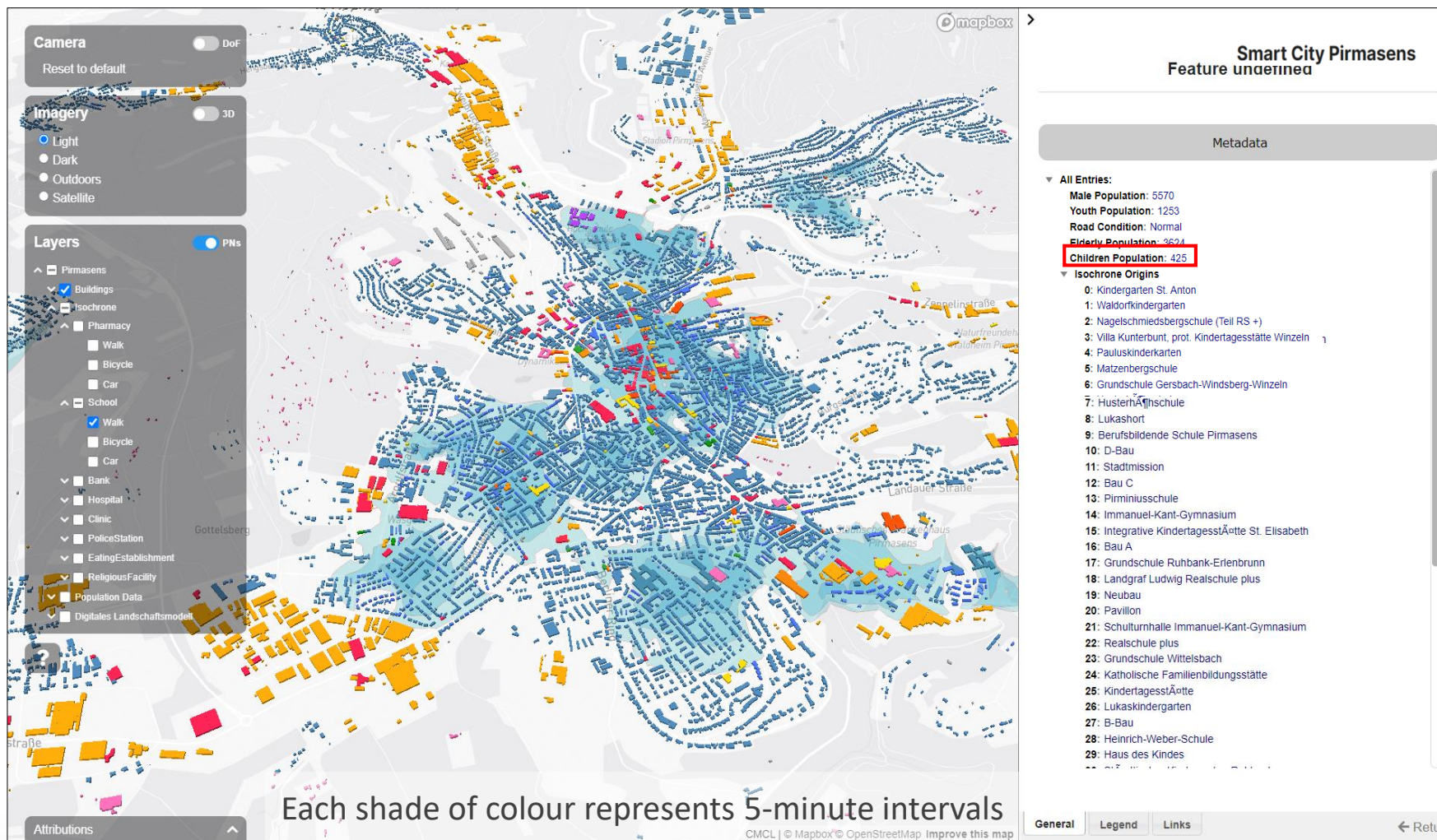


The World Avatar (TWA)

Isochrone map for all schools in Pirmasens

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

Scale - City



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

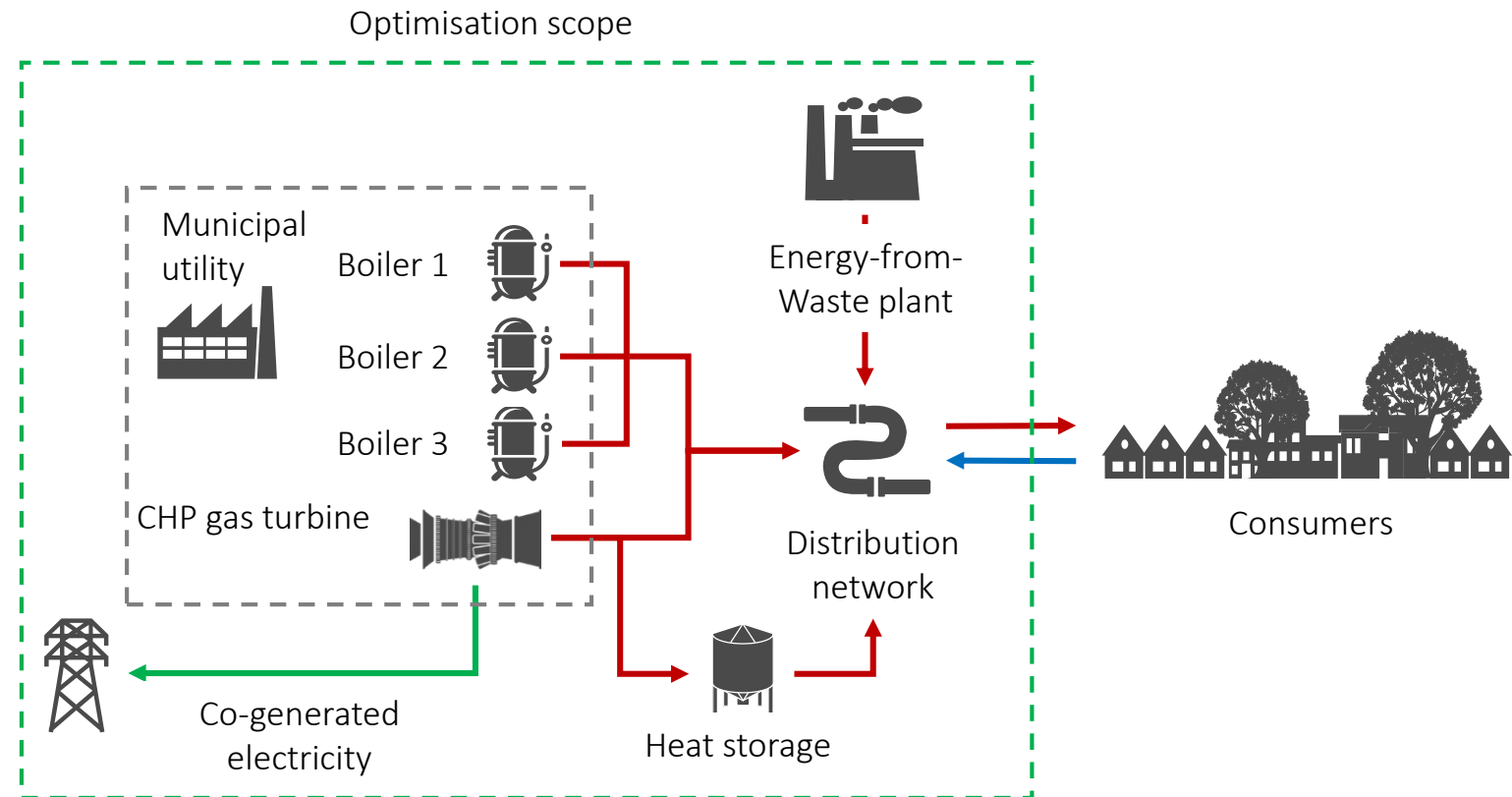
Scale - City

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

Continuous data
integration

- Gas price
- CO₂ price
- Electricity spot price
- Temperature

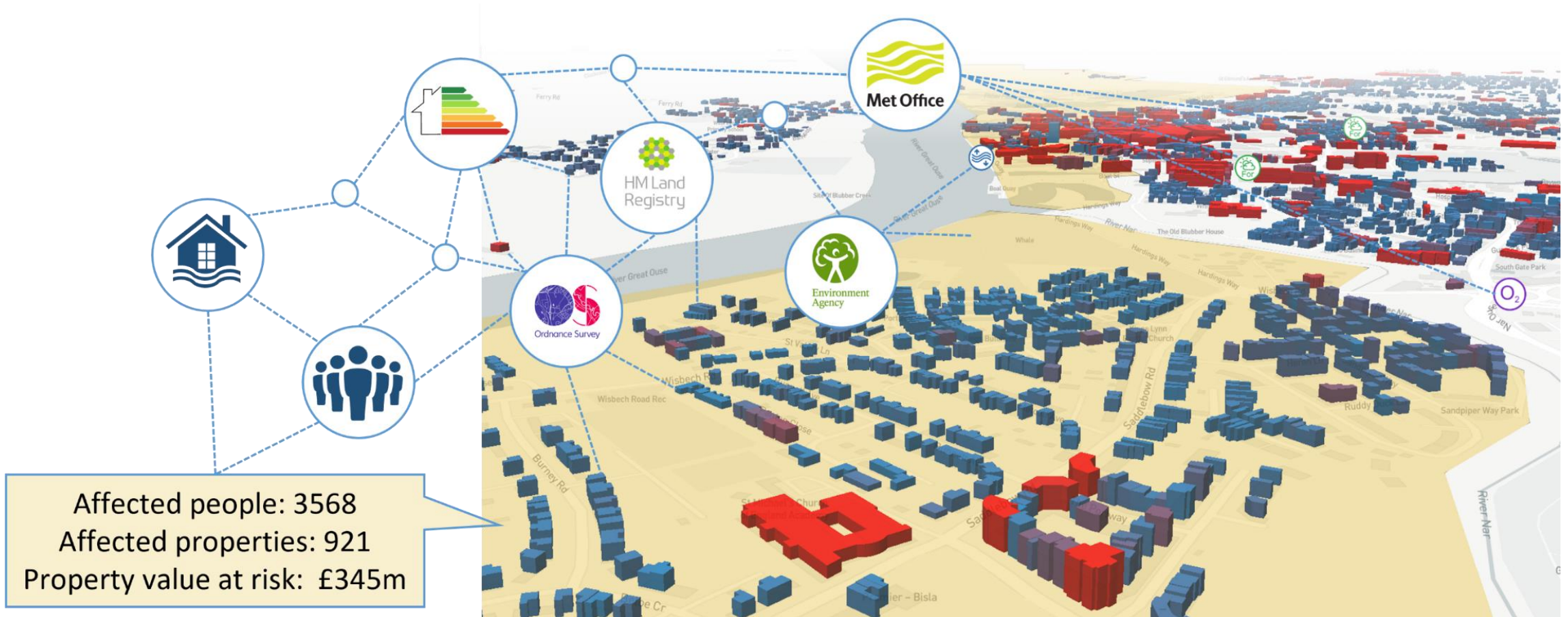
- Heat demand
- Flow temperatures
- Return temperatures



<https://doi.org/10.1016/j.apenergy.2021.117877>

The World Avatar (TWA)

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



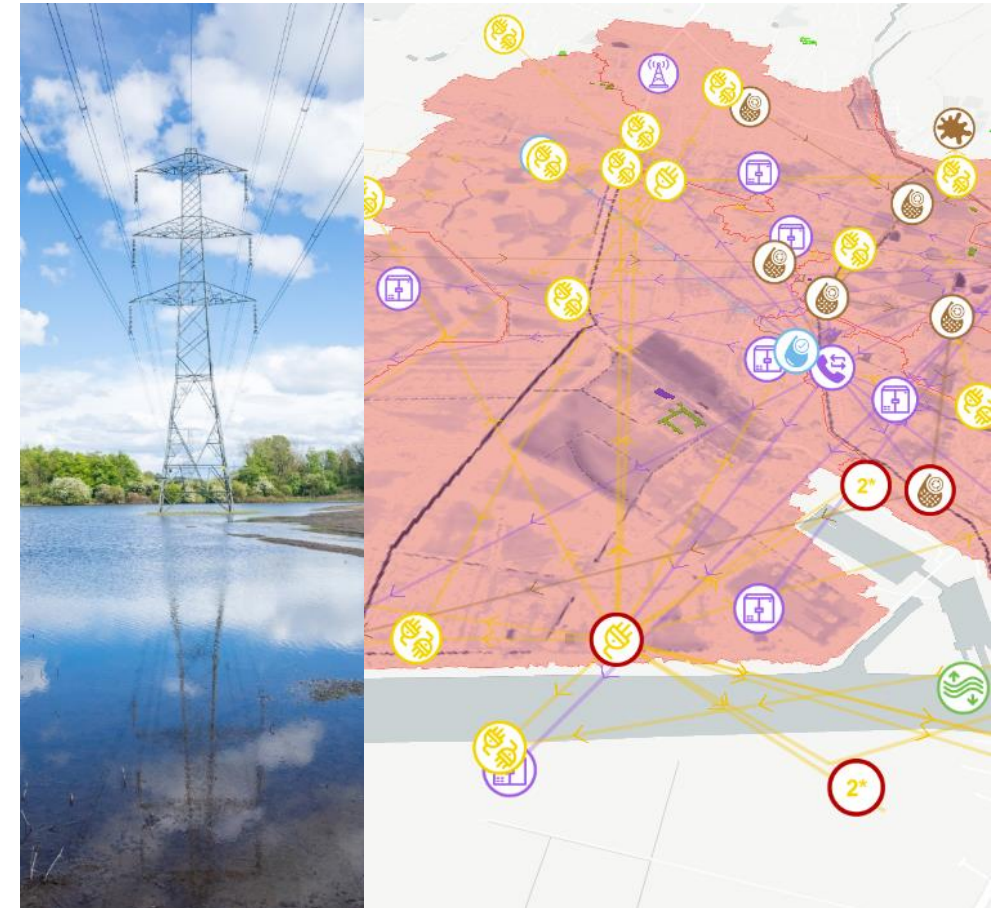
The World Avatar (TWA) Climate Resilience Demonstrator (CReDo)

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



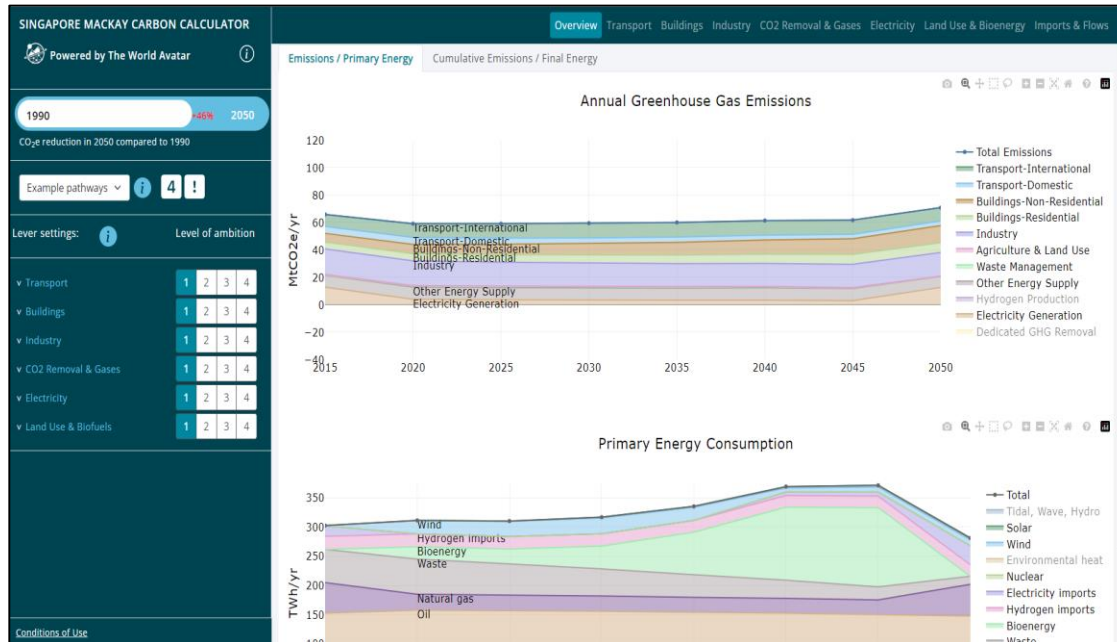
A real-life flooding event and a simulated example using the CReDo visualisation tool

The World Avatar (TWA)

Singapore MacKay Carbon Calculator

Scale - Country

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						
Lighting - Residential	Index	1.00	1.50	1.00	0.85	0.70
Lighting - Non-Res	Index	1.00	1.30	1.00	0.75	0.50
Appliance - Residential	Index	1.00	1.50	1.00	0.75	0.50
Appliance - Non-Res	Index	1.00	1.30	1.00	0.90	0.80
Energy Intensity						
Lighting - Residential	Index	1.00	0.75	0.33	0.33	0.25
Lighting - Non-Res	Index	1.00	0.75	0.50	0.50	0.40
Appliance - Residential	Index	1.00	0.90	0.77	0.63	0.50
Appliance - Non-Res	Index	1.00	0.90	0.77	0.63	0.50
Air Con - Residential	Index	1.00	0.90	0.77	0.63	0.50
Air Con - Non-Res	Index	1.00	0.90	0.77	0.63	0.50

Residence Appliance - Energy Intensity Index

Expansion to Singapore context

Dynamic data incorporation

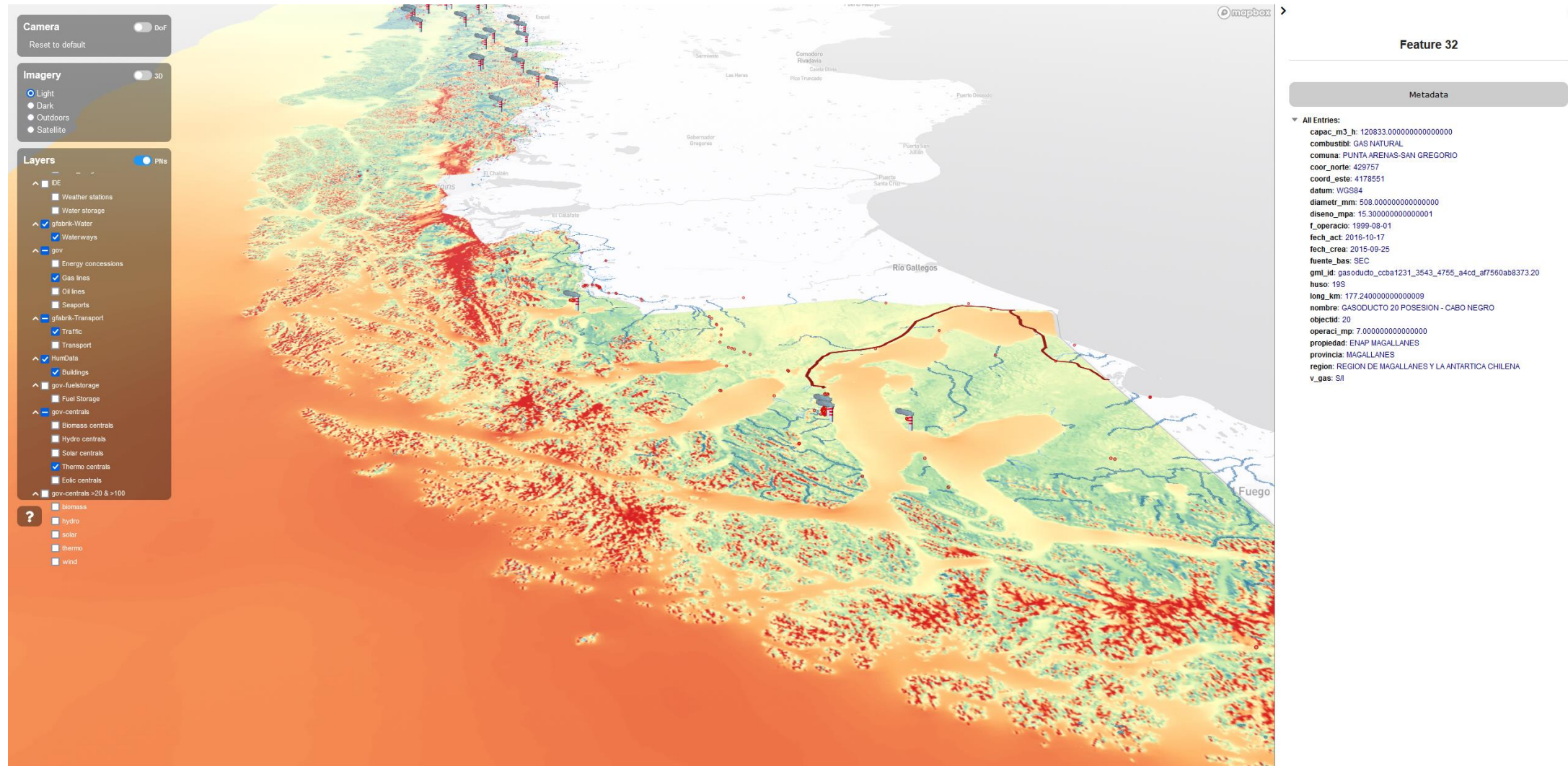
2050 Net Zero path optimizer

Any Location

The World Avatar (TWA)

Representation of cross-domain data in Chile

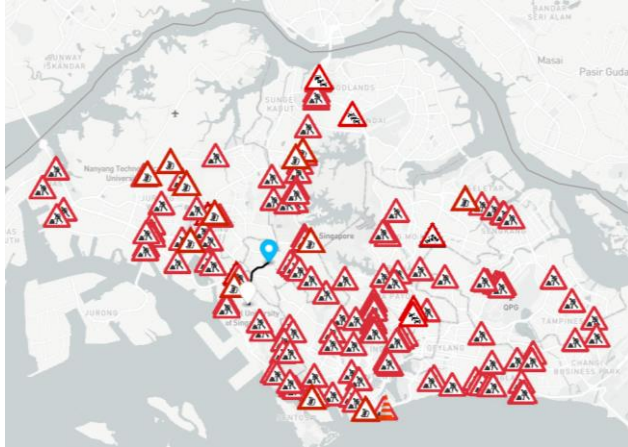
Scale - Country



The World Avatar (TWA)

Applicable and extendable to any location

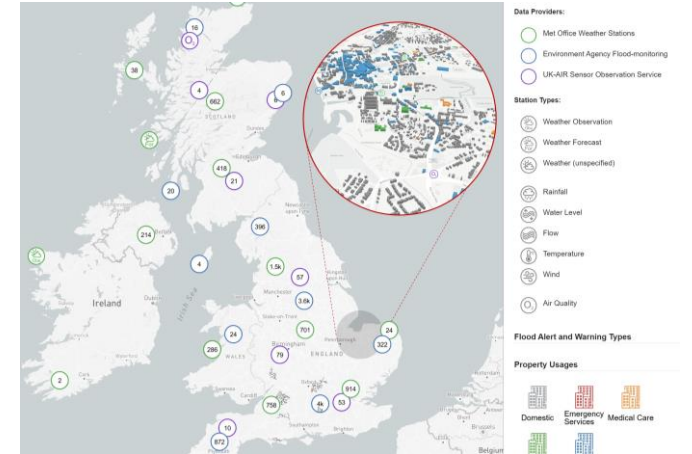
Singapore



The World Avatar

Any Location

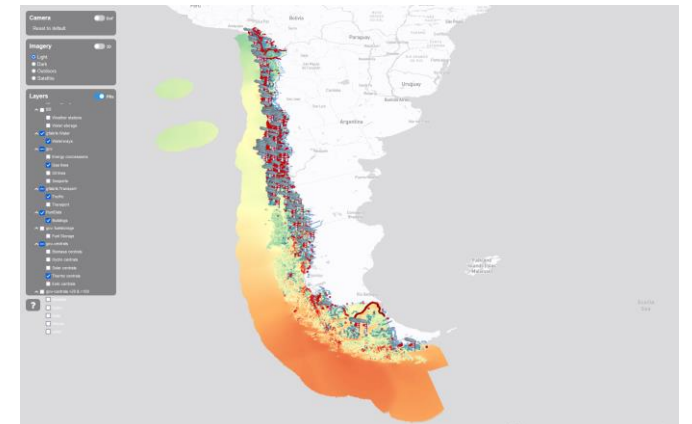
UK



Germany



Chile

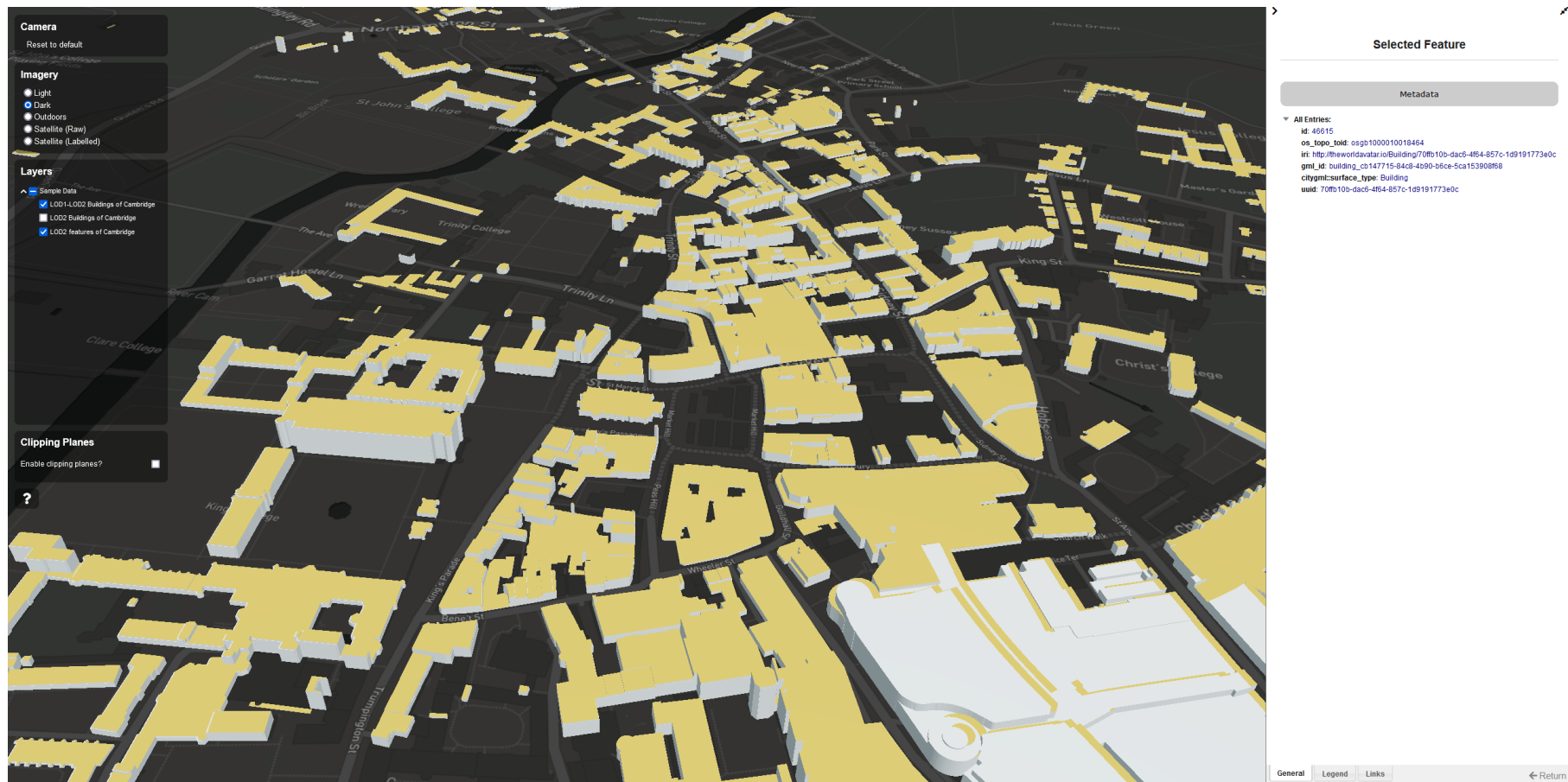


Interfaces

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



The World Avatar (TWA)

Unified User Interfaces

Mobile App and Dashboard

