34th Annual INCOSE international symposium
hybrid event
Dublin, Ireland
July 2 - 6, 2024

Expanding Horizons with Graph Embeddings to understand large trade space from generative methods

Trade Space Wonders

Mike Nicolai, Kefan Sun, Clement Bertheaume, Siemens

Agenda

- **Introduction** — Generative methods, challenge, objective
- **Technical Details** — Methodology explained with a toy example
- **Results** — Real-world use cases, evaluation method, findings
- **Conclusion** — Takeaways

Introduction

Trade Studies in Practice

- Do you do trade studies ?

- How many variants or architectures do you investigate?

The promised land of Generative

Product R&D: Reducing research and design time, improving simulation and testing

Continue to next section

Share

Potential productivity lift
Product R&D

12%
of global functional spending

~$328B

Generative AI's potential in R&D is perhaps less well recognized than its potential in other business functions. Still, our research indicates the technology could deliver productivity with a value ranging from 10 to 15 percent of overall R&D costs.

For example, the life sciences and chemical industries have begun using generative AI foundation models in their R&D for what is known as generative design. Foundation models can generate candidate molecules, accelerating the process of developing new drugs and materials. Entos, a biotech pharmaceutical company, has paired generative AI with automated synthetic development tools to design small-molecule therapeutics. But the same principles can be applied to the design of many other products, including larger-scale physical products and electrical circuits, among others.

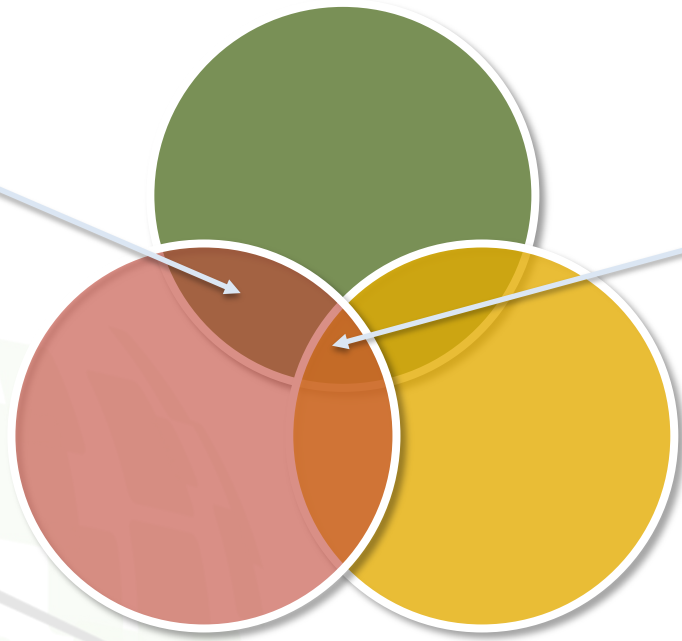
While other generative design techniques have already unlocked some of the

Automatic Trade Space Generation

Generative Methods

Rule-based
Procedural modelling

Commercially available in
Simcenter Studio



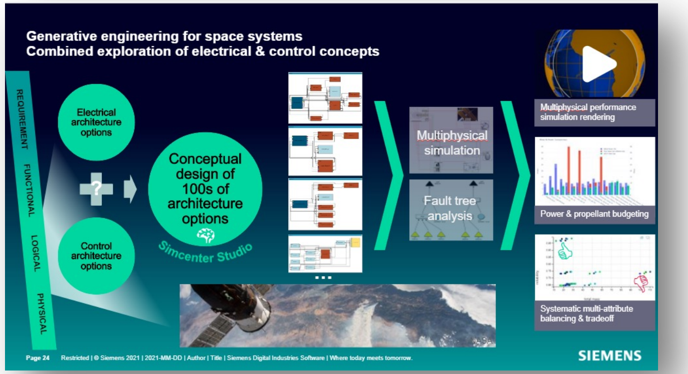
Existing research prototype, more semantic understanding needed for LLM to create meaningful output

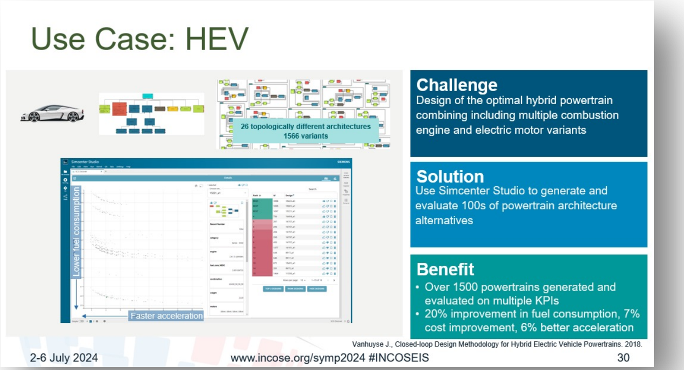
Declarative
Computational design synthesis

Data-driven
Generative AI

Use Case Overview

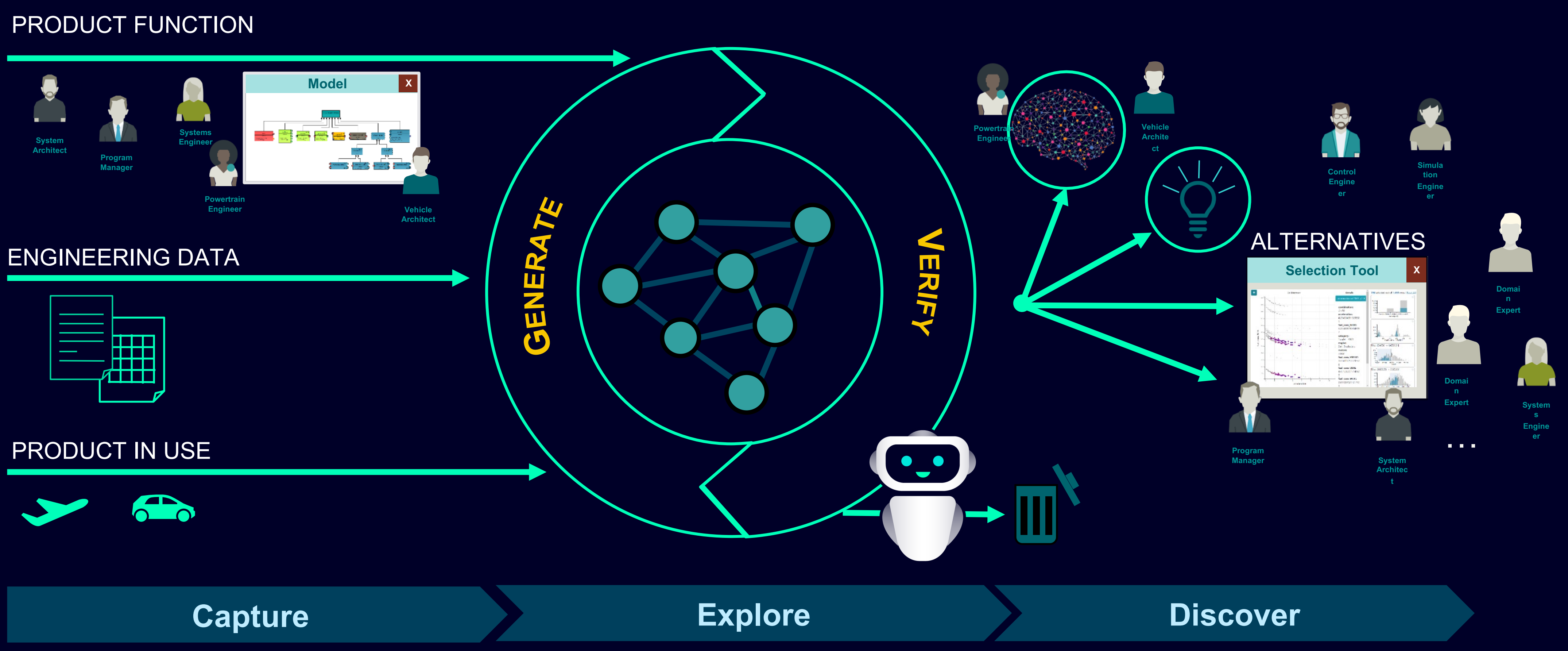
Use Case	Type	# Architectures	# Variants
APOLLO	Mission	15	108
FIRESAT	System	8	56
HEV	Subsystem	26	1566
HEV benchmark	Subsystem	26 - 48968	1 per architecture





Automatic Systems Architecture Creation and optimization

From a Function to Logic Architecture



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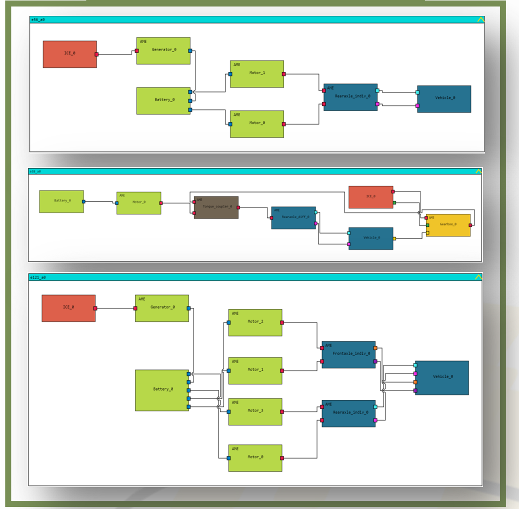
Objectives

- **Understand** and **navigate** the design space
- **Unsupervised**: No labels required
- Encode **structural** and **parametric** information
- Create vector representation (**embeddings**) of designs
- Explore **similarity** and **dissimilarity** of designs
- **Interpretation** similar to human understanding

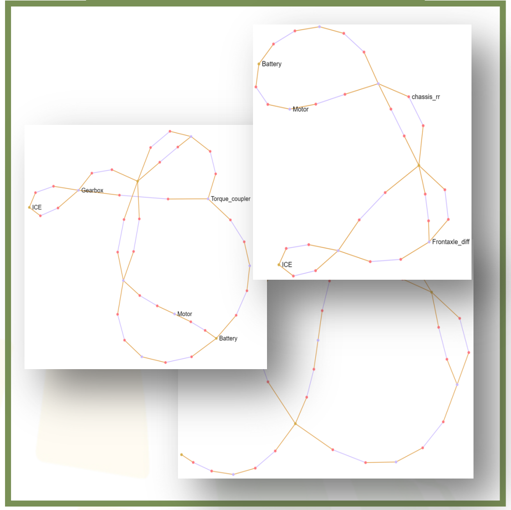
Technical Details

Method Outline

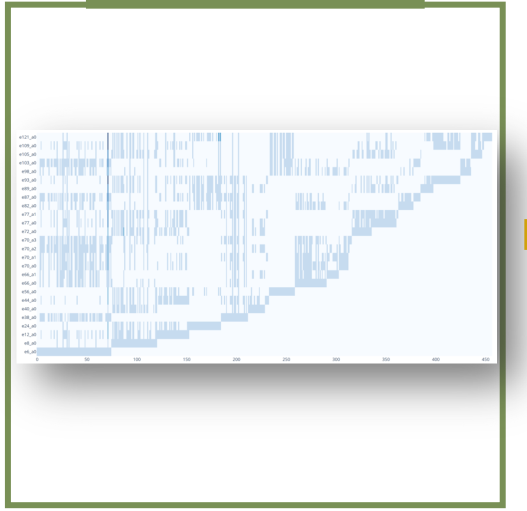
Generated Architectures



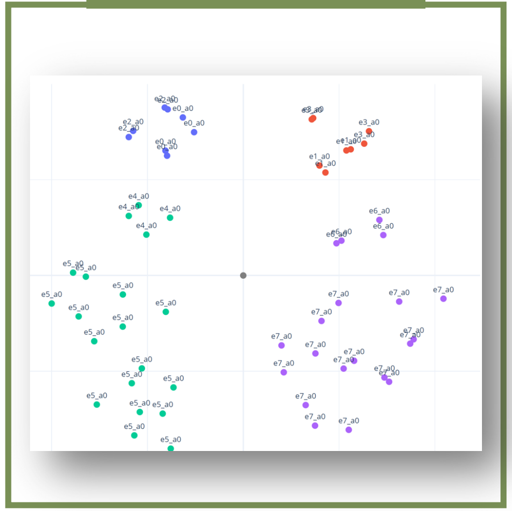
Graphs



Embeddings



Reduced Embeddings



(1)

Data Preprocessing

(2)

Graph Embedding

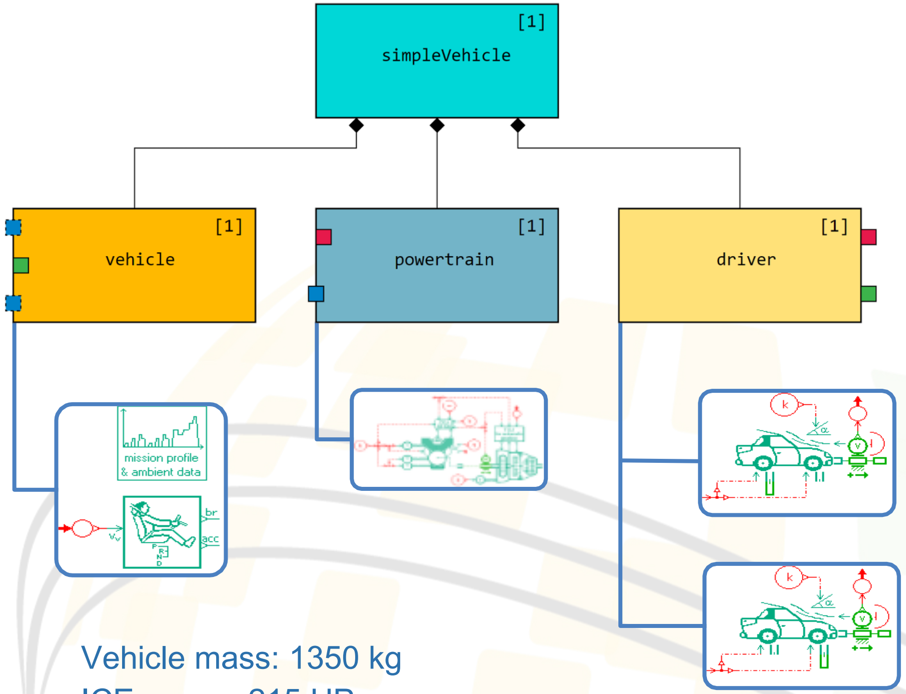
(3)

Dimensionality Reduction

Toy Example

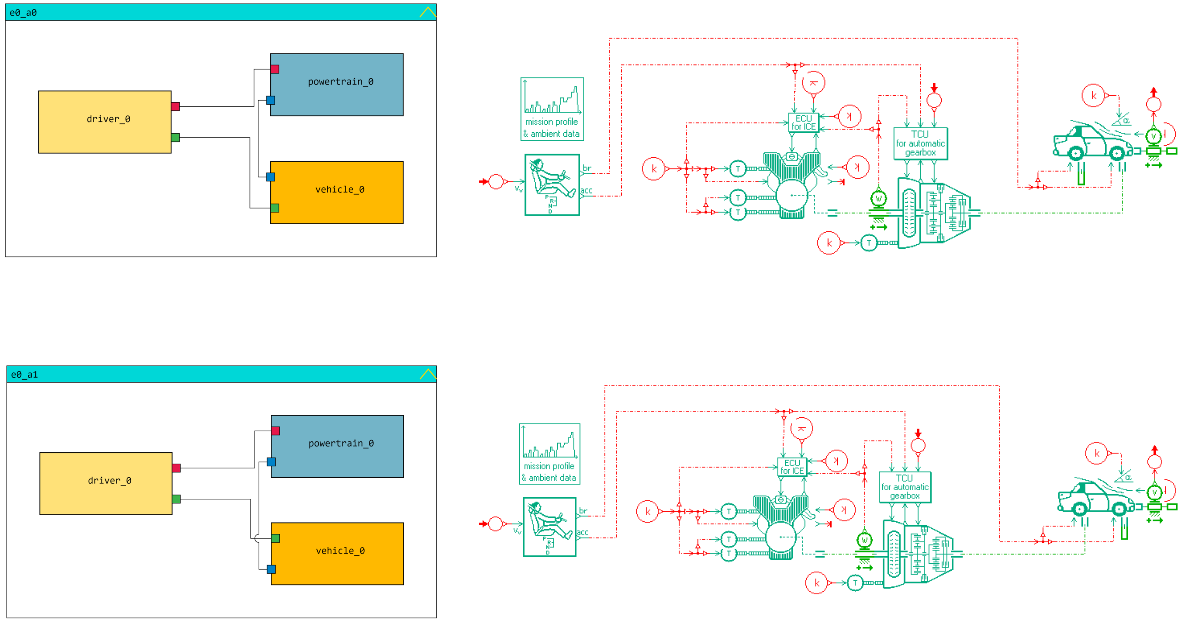
Note:
Toy example for illustrative purpose,
method scales to hundreds of components.

System Model



Vehicle mass: 1350 kg
ICE power: 215 HP
Weight distribution: 55%
Tires: 175/70R14
Friction coefficient: 0.8

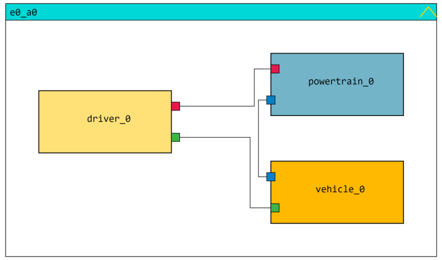
Generated Architectures



Data Preprocessing

All information is preserved.

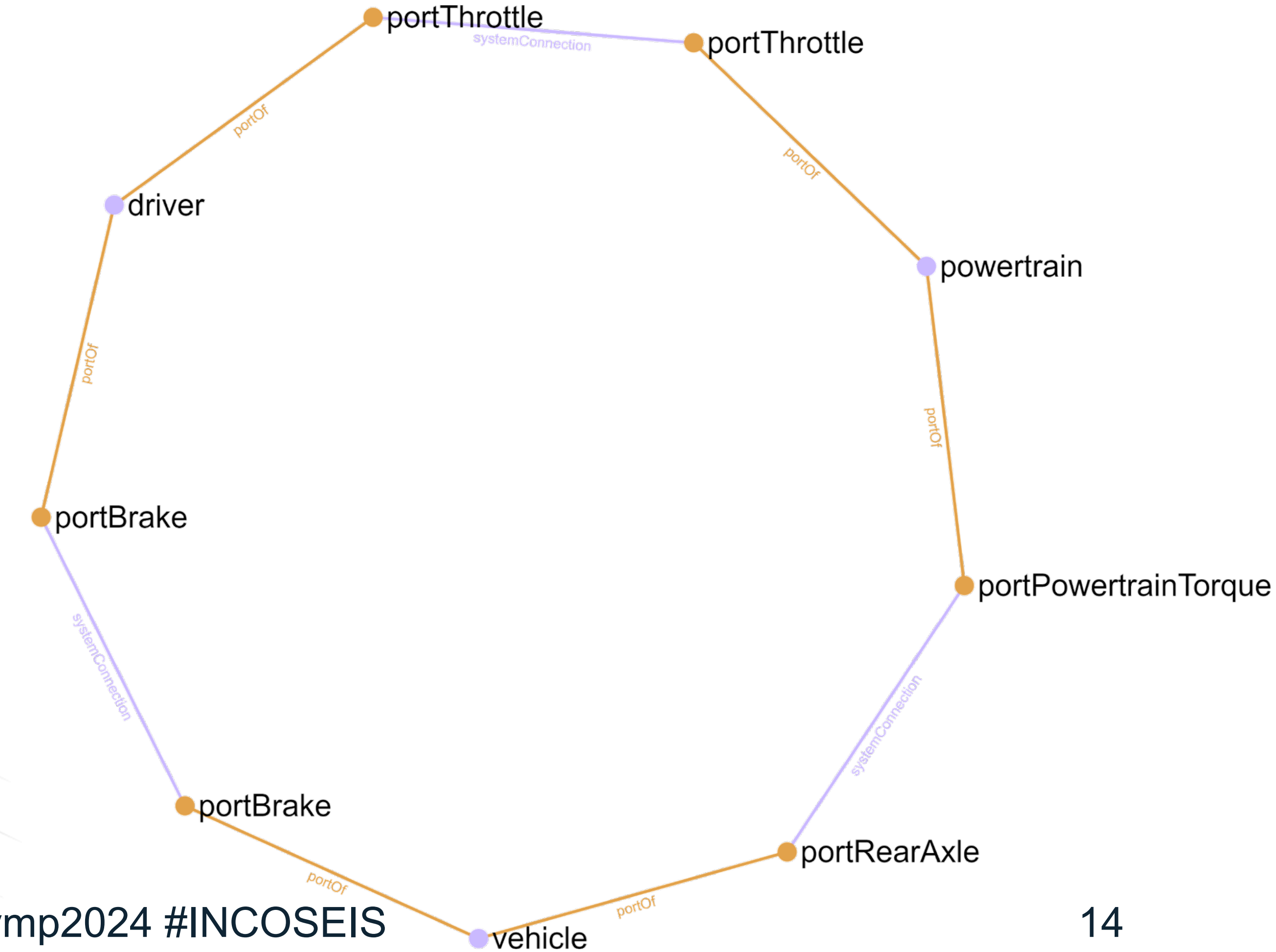
Generated Architectures



Vehicle mass: 1350 kg
ICE power: 215 HP
Weight distribution: 55%
Tires: 175/70R14
Friction coefficient: 0.8

Graphs

Components and ports as nodes
Relationships as edges
Parameters as node attributes



Graph Embeddings

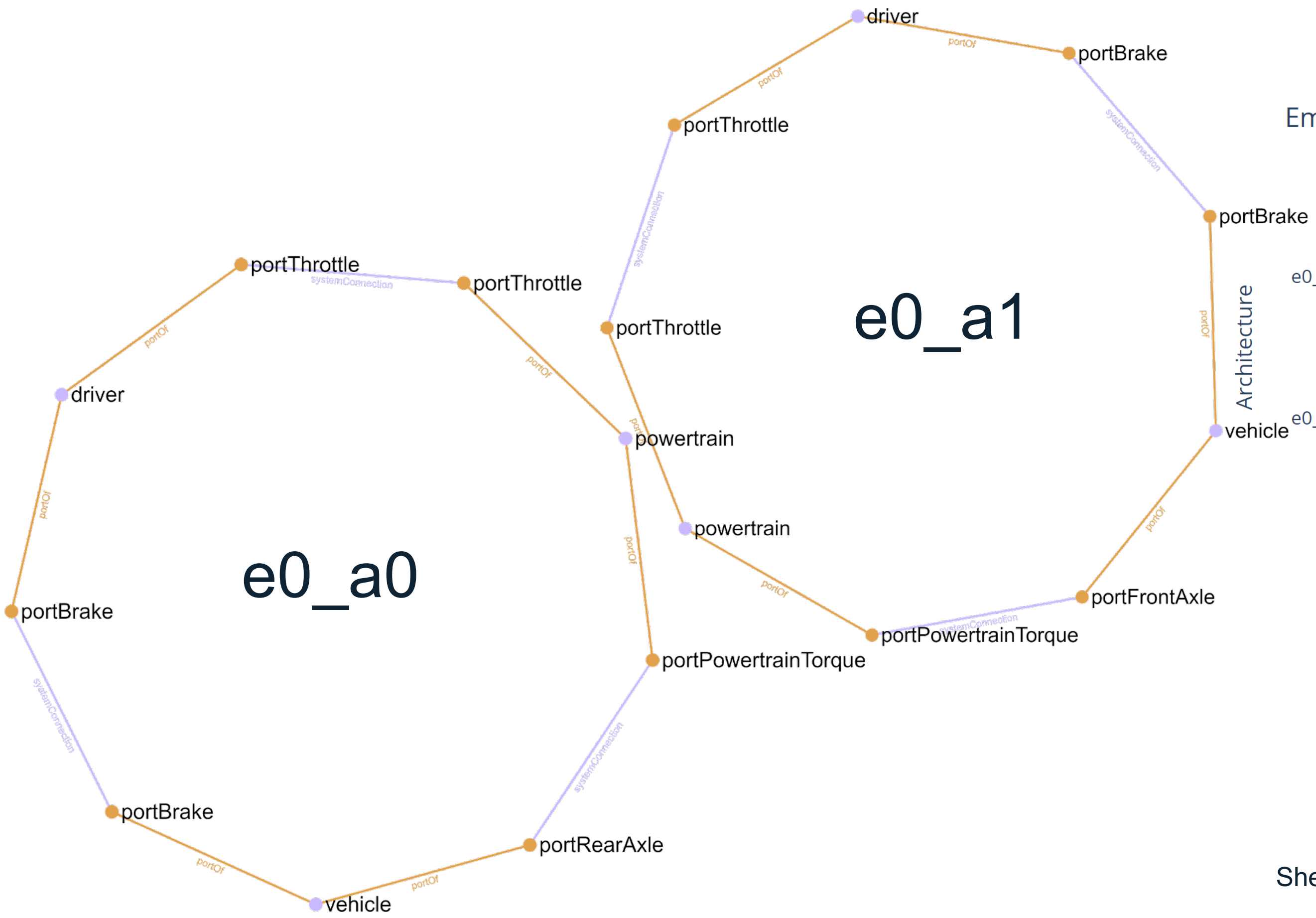
All information is preserved.

Graphs

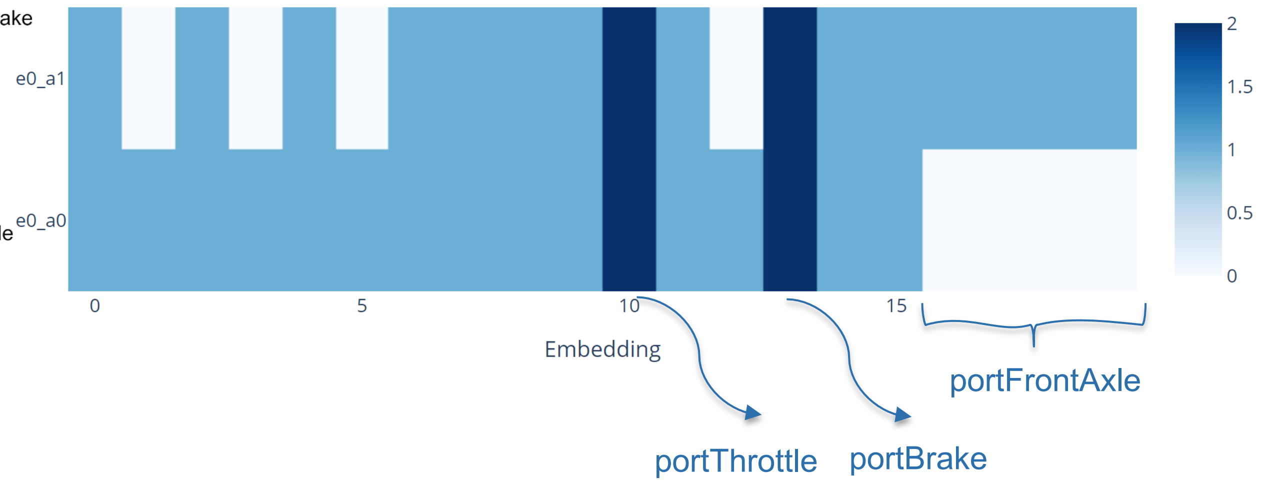
Components and ports as nodes
Relationships as edges
Parameters as node attributes

Embeddings

Counting: simple, fast, explainable
Node and edge attributes
Sparse, big matrix



Embedding matrix for simpleVehicle (Weisfeiler Lehman graph kernel with iteration = 1)



Shervashidze, N. et al., Weisfeiler Lehman Graph Kernels. Journal of Machine Learning Research. 2011.

Dimensionality Reduction

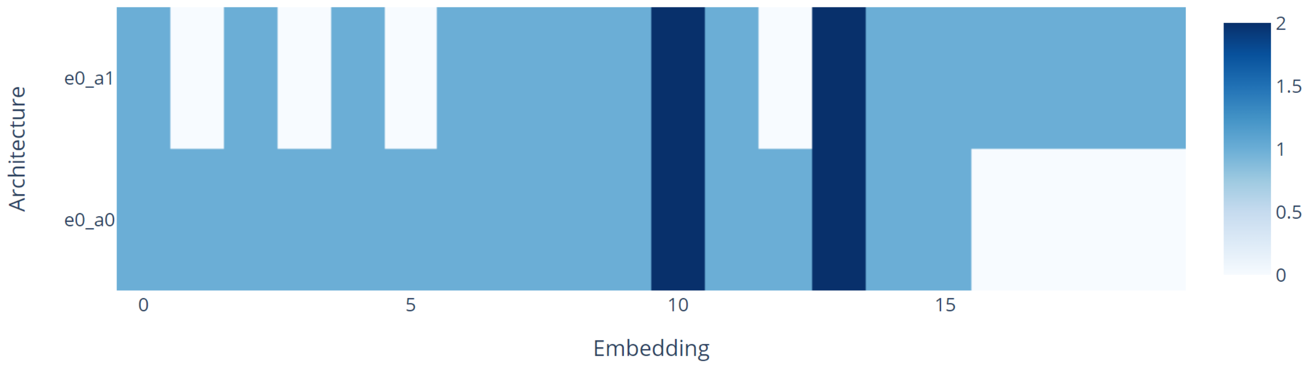
Embeddings

Counting: simple, fast, explainable
Node and edge attributes
Sparse, big matrix

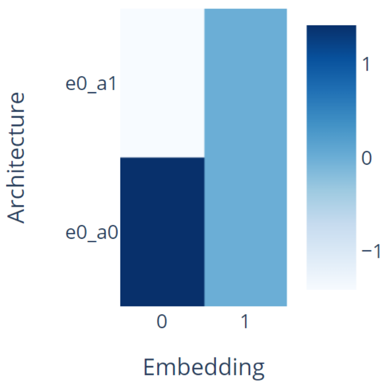
Reduced Embeddings

Coordinates of design architectures
Similarity and dissimilarity
Dense, small matrix

Embedding matrix for simpleVehicle (Weisfeiler Lehman graph kernel with iteration = 1)



Reduced embedding matrix for simpleVehicle (Weisfeiler Lehman graph kernel with iteration = 1)



Dimensionality Reduction

Embeddings

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Node and edge attributes
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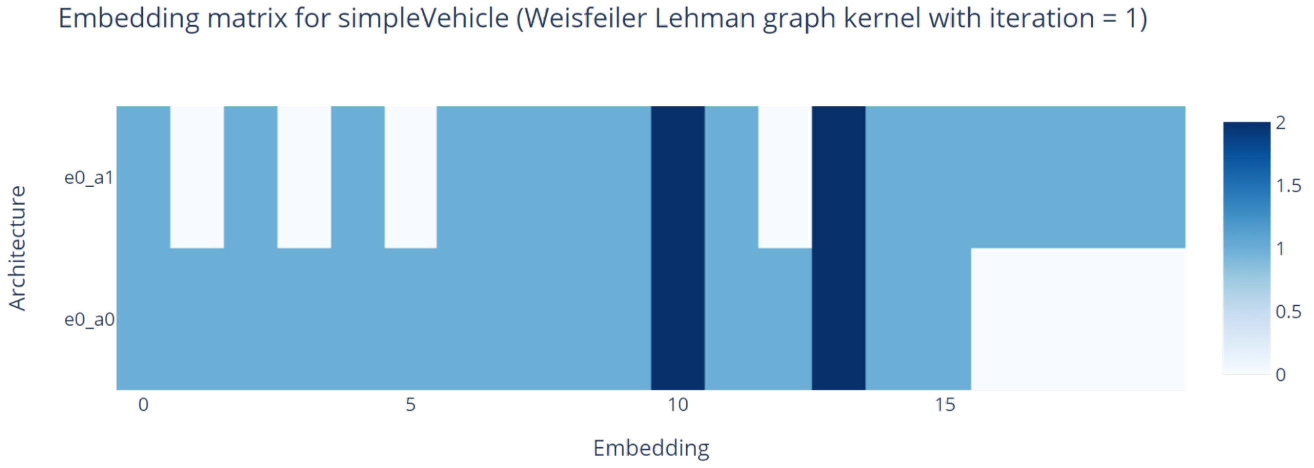
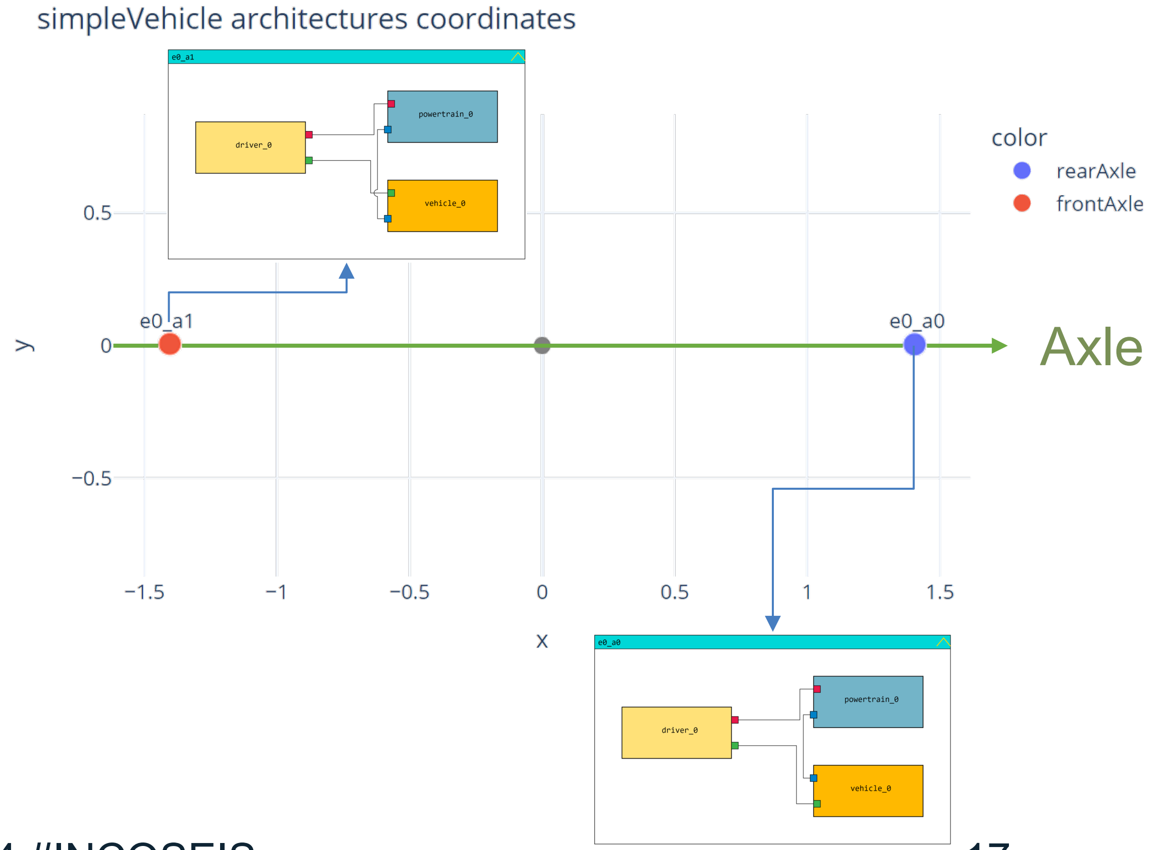




Results

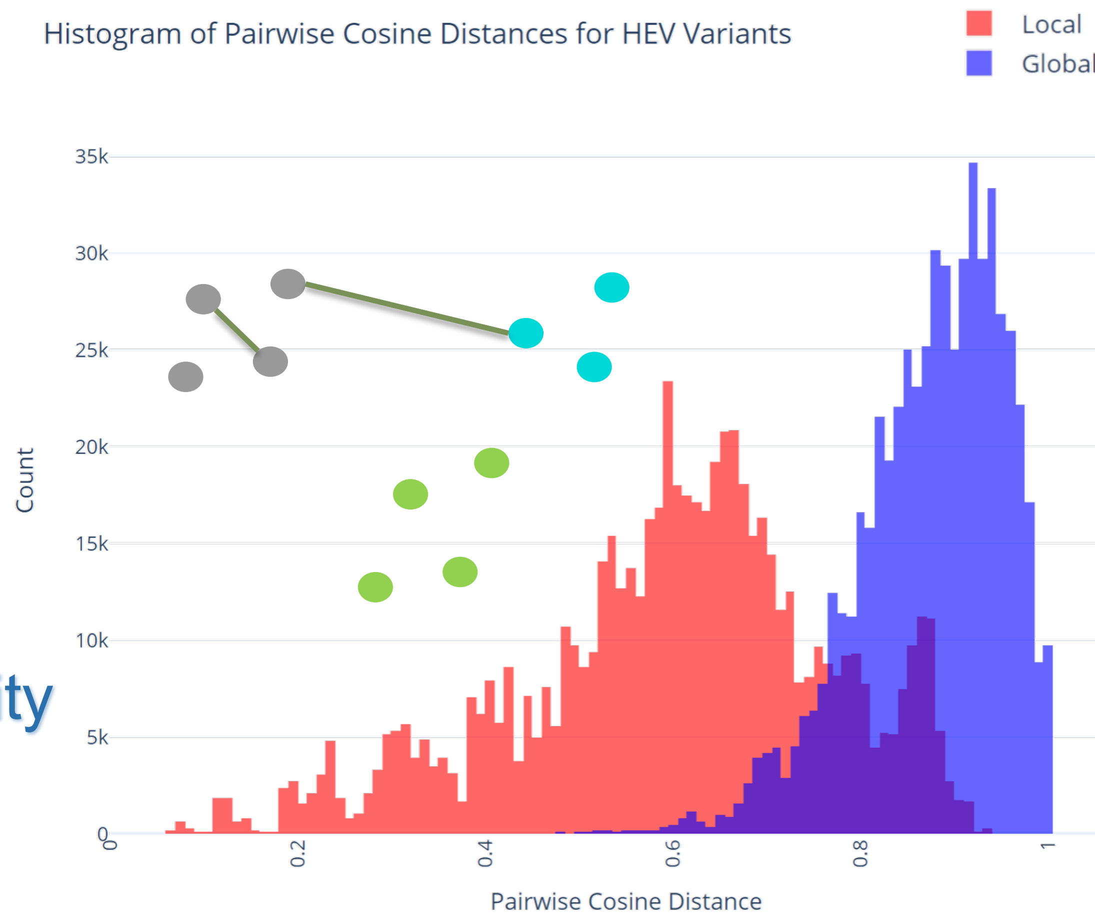
Evaluation Method

Embedding Space

- **Labels**: Domain knowledge and human interpretation
- **Local Structure**: Intra-cluster structure characterized by local distance – intra-cluster pairwise distance
- **Global Structure**: Inter-cluster structure characterized by global distance – inter-cluster pairwise distance

Similarity

Dissimilarity



Kolmogorov-Smirnov test:

Use Case	Statistic	P-value
APOLLO	0.46	8e-05
APOLLO Variants	0.63	4e-07
FIRESAT	0.83	7e-03
FIRESAT Variants	0.80	8e-216
HEV	0.73	3e-36
HEV Variants	0.75	0.0

Conclusion: For all use cases, there is a statistically significant difference between the local and global distributions.

Evaluation Method

Dimensionality Reduction (DR)

Method	Year	Type
MDS	1964	Exact
PaCMAP	2021	Approximate
PCA	1901	Projection

Reduced Space

Qualitative:
- Visual inspection of design coordinates

Quantitative:
- **Baseline**: Original embedding space
- **Local Structure**: Let d be a design in the reduced space T, y its true label, and $\tilde{y}$ the label predicted by a k-nearest neighbor classifier. The accuracy is given by:

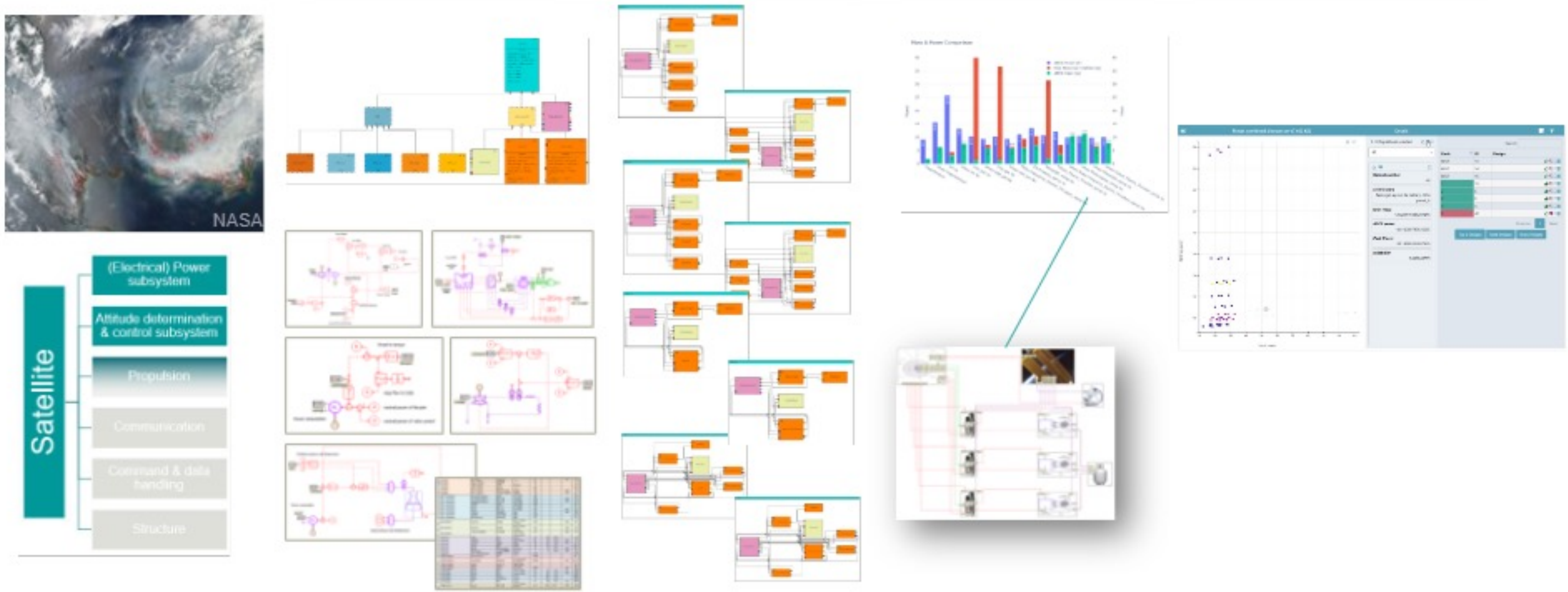
$$KNN = \frac{1}{|T|} \sum_{d \in T} 1(y = \tilde{y})$$

- **Global Structure**: Random Triplet Accuracy (RTA).

Kruskal, J.B., Multidimensional Scaling by Optimizing Goodness of Fit to a Nonmetric Hypothesis. Psychometrika. 1964.
Wang, Y. et al., Understanding How Dimension Reduction Tools Work: An Empirical Approach to Deciphering t-SNE, UMAP, TriMAP, and PaCMAP for Data Visualization. Journal of Machine Learning Research. 2021.
Pearson, K., On Lines and Planes of Closest Fit to Systems of Points in Space. Philosophical Magazine. 1901.

Use Case: FIRESAT

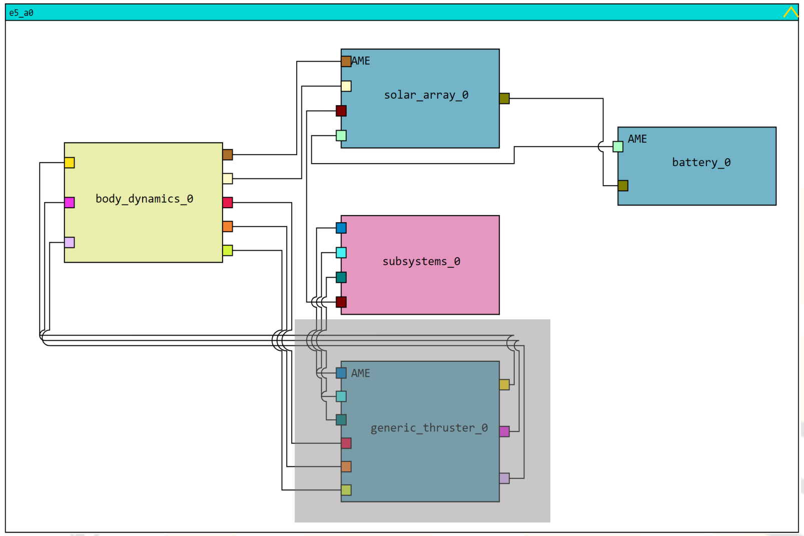
Mission design & objective → Subsystems definition, asset library → Architecture & configuration generation → Simulation & postprocessing → Attribute balancing & solution selection

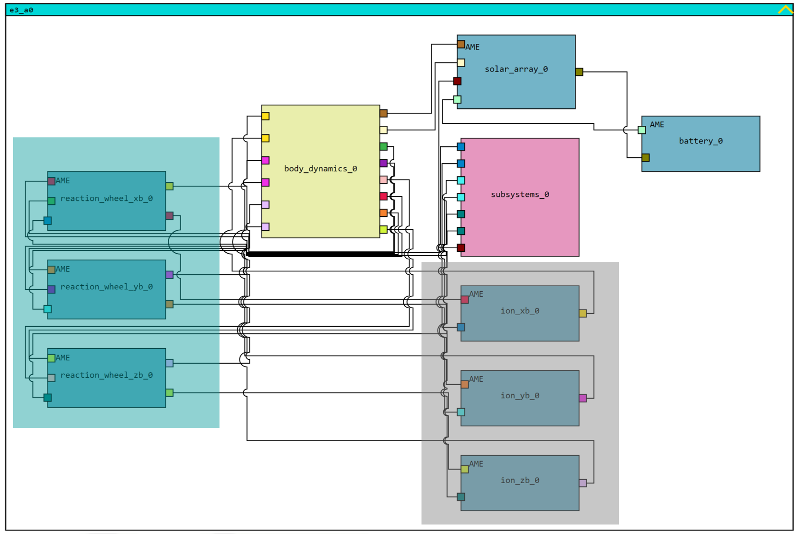


Use Case: FIRESAT

Architectures

8 Architectures





Variants

56 Variants

- Solar array: Si or GaAS MJ
- Battery: NiCa or NiHy
- Generic thruster: 1, 2, 3, 4

Use Case: FIRESAT

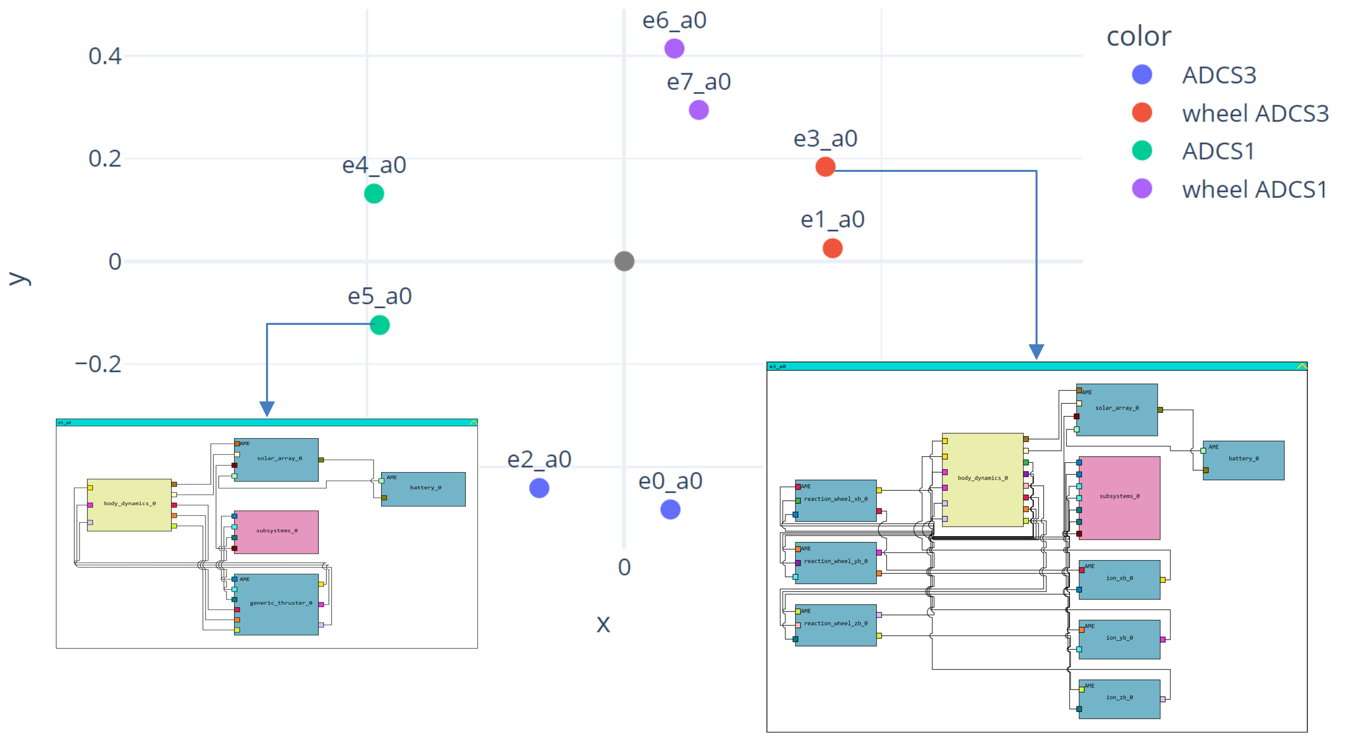
Architectures

y = x for ADCS
y = -x for reaction wheel

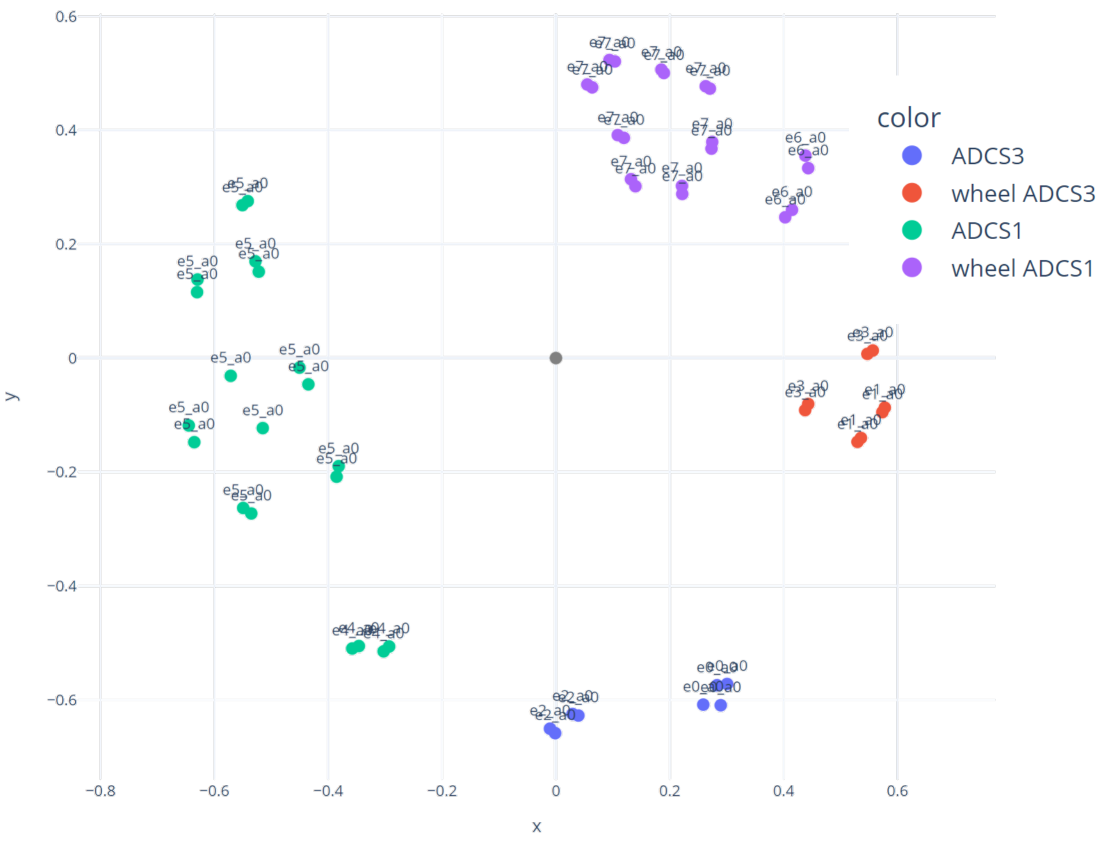
Variants

Clusters further expanded
Relative positions preserved

FIRESAT architectures coordinates - MDS

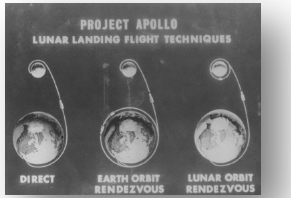


FIRESAT variants coordinates - MDS



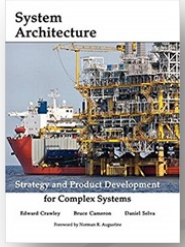
Use Case: APOLLO

Capture | **Explore** | **Discover**

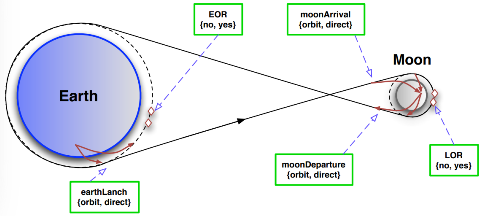


Considered 1962:

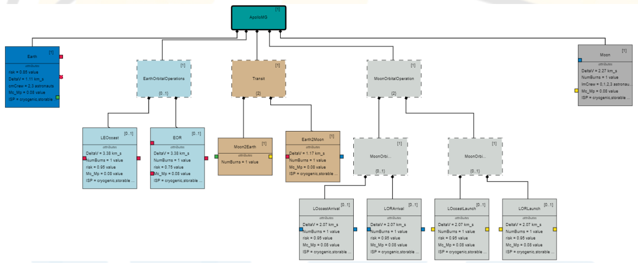
- Earth Orbit Rendezvous (EOR)
- Lunar Orbit Rendezvous (LOR)
- Liquid Nova Direct (NOVA DF)
- Saturn C-5 Direct (C-5 DF)

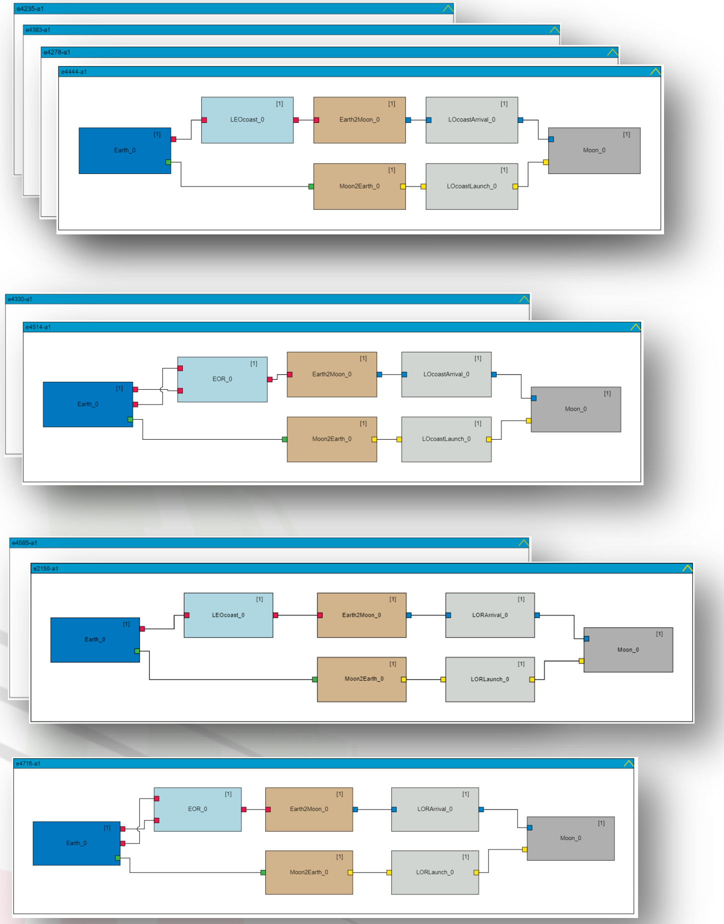


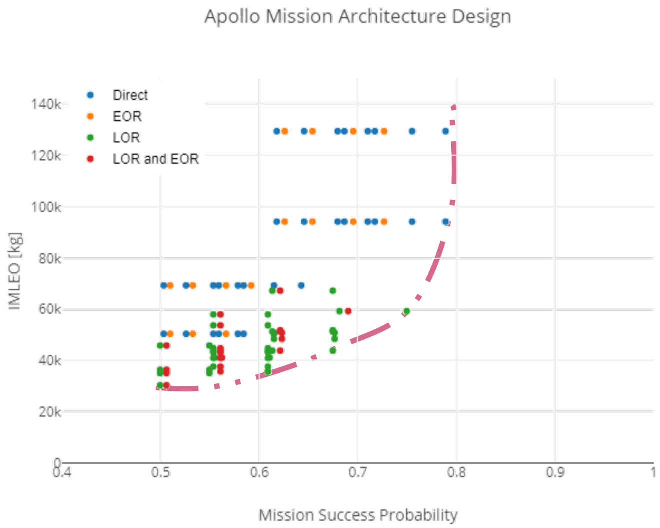
Nowadays part of textbooks



Remodeled with Simcenter Studio:







Trade-study considering:

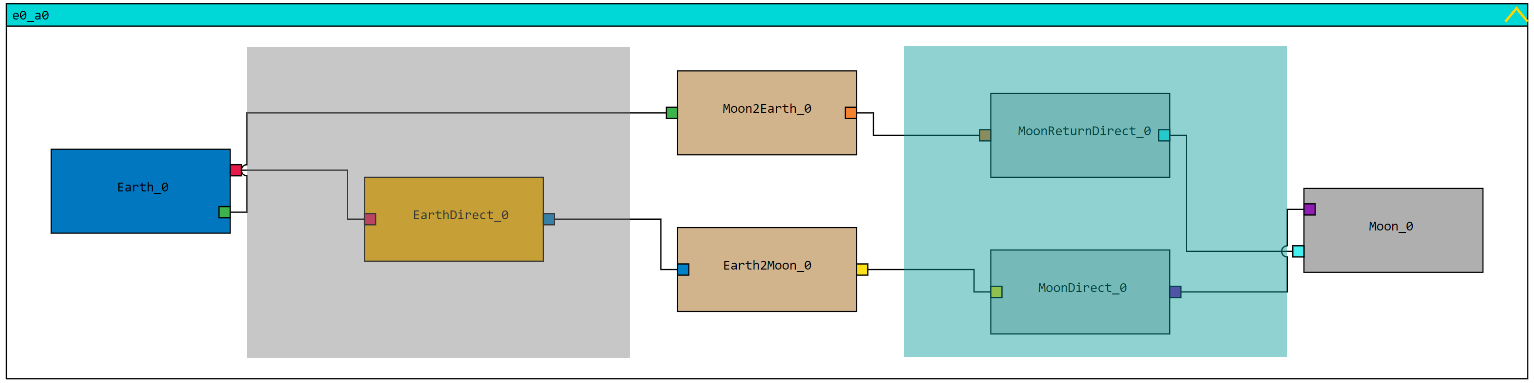
- Architecture
- Crew size
- Propellant type
- Number of burns

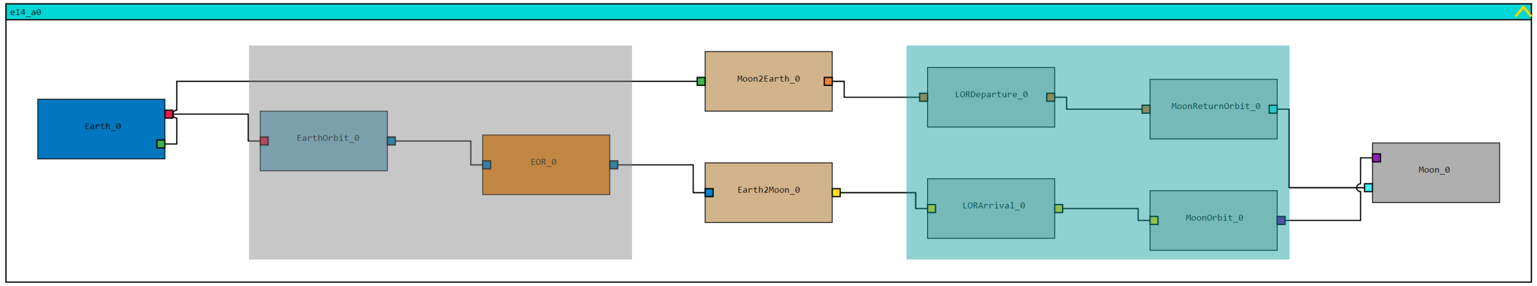
Use Case: APOLLO

Architectures

Variants

15 Architectures





108 Variants

- # Crew Members: 2, 3
- # Crew Members to Moon: 1, …, all
- Fuel Type: storable and/or cryogenic

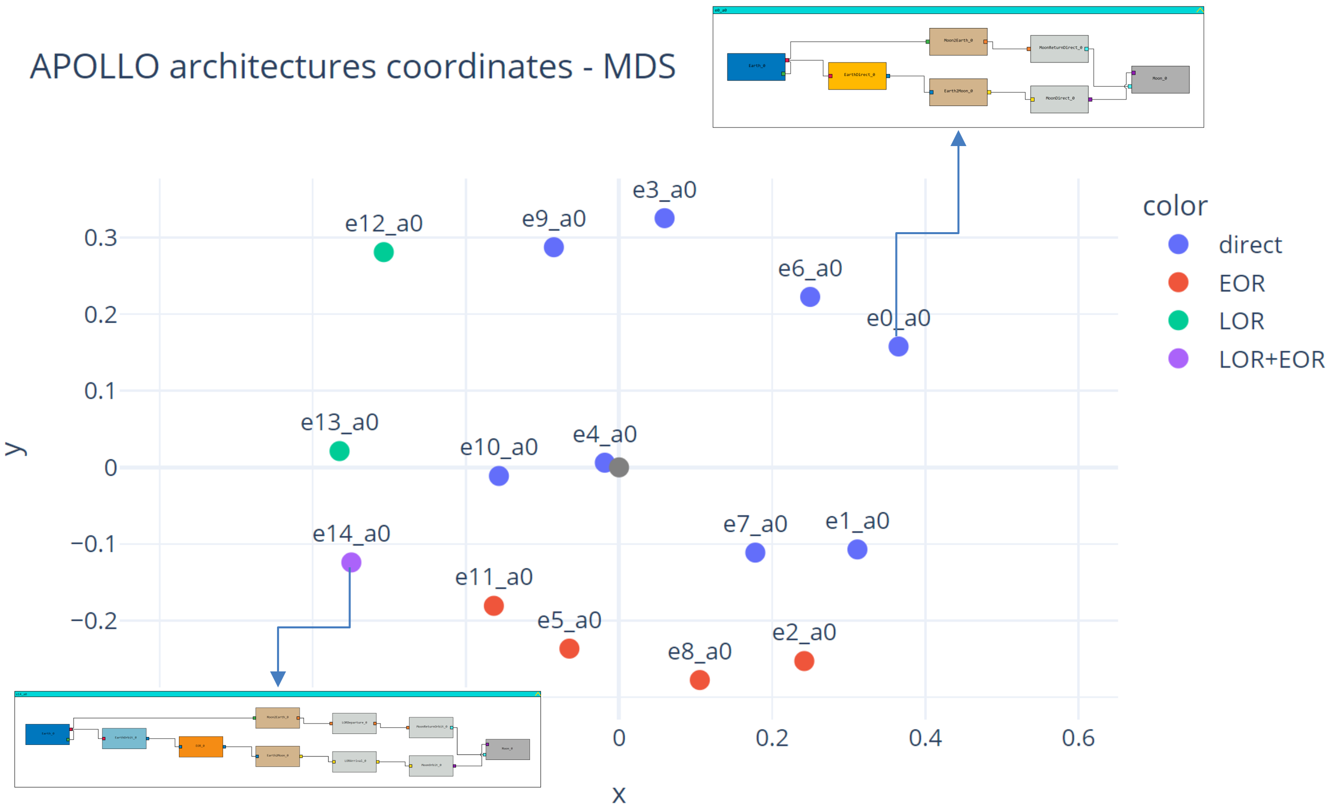
Use Case: APOLLO

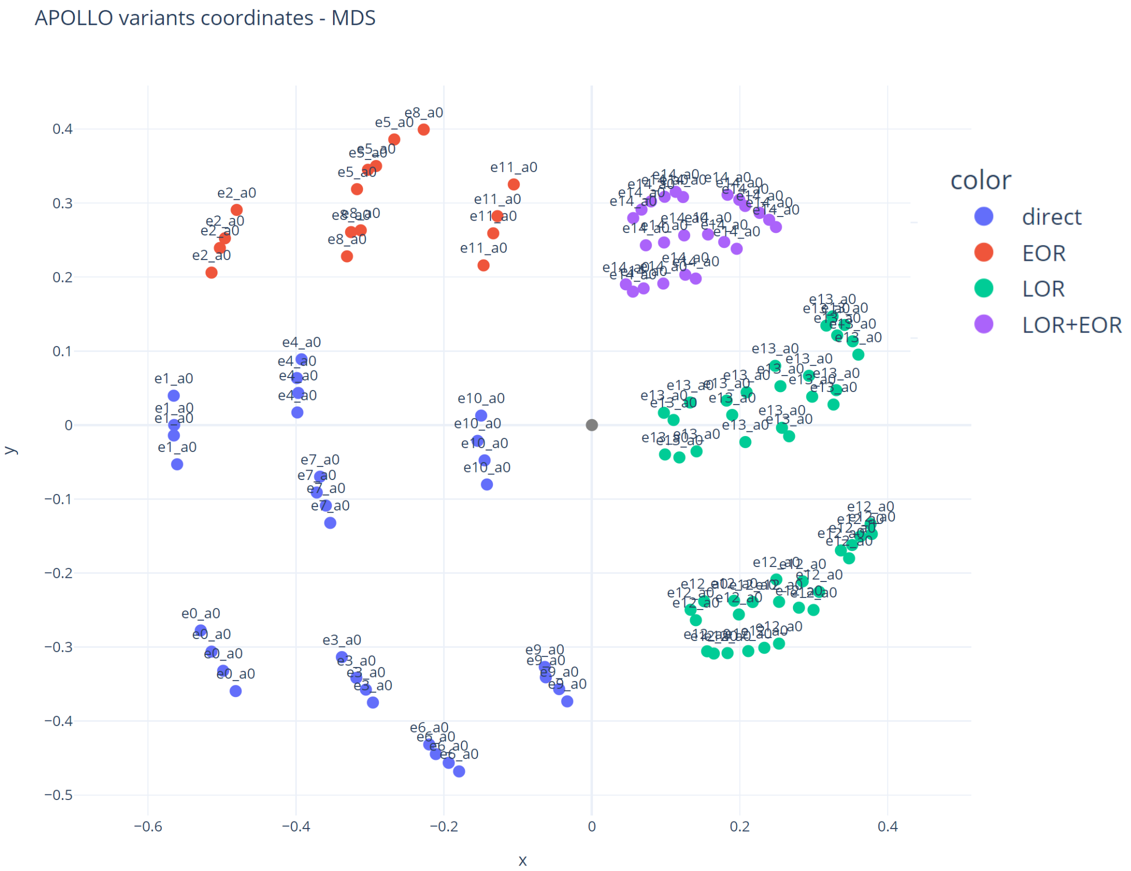
Architectures

X-axis for LOR
Y-axis for EOR

Variants

Clusters further expanded
Relative positions preserved





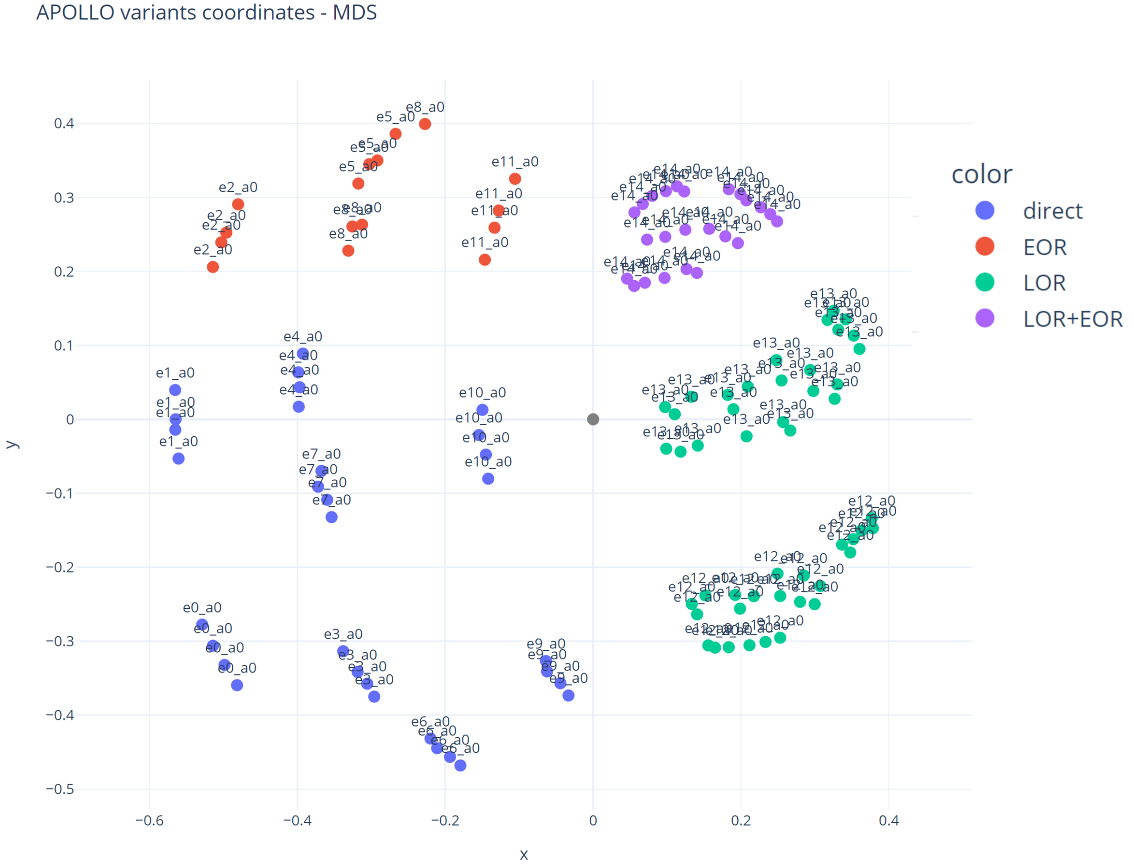
Use Case: APOLLO – DR Comparison

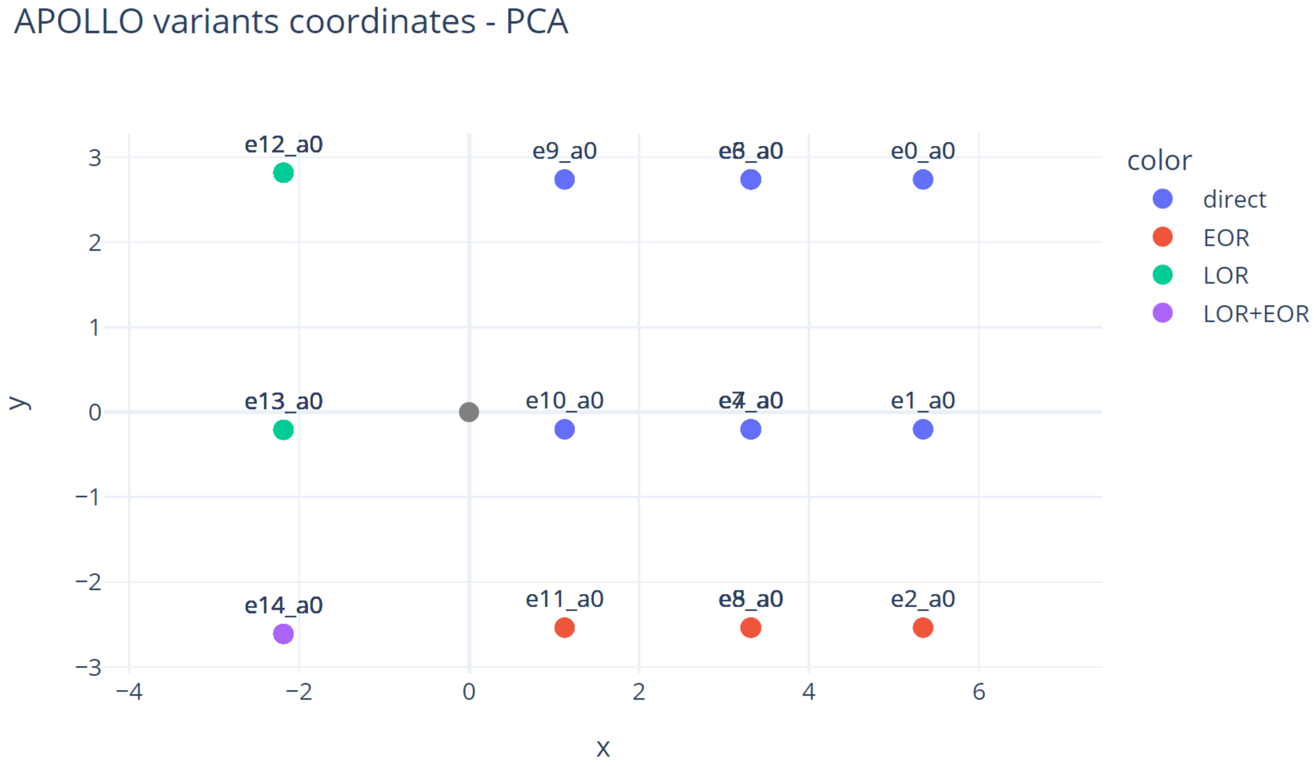
Variants

Clusters further expanded
Relative positions preserved

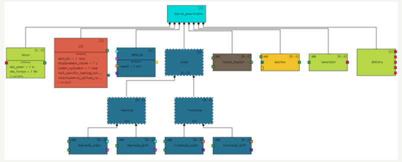
Variants

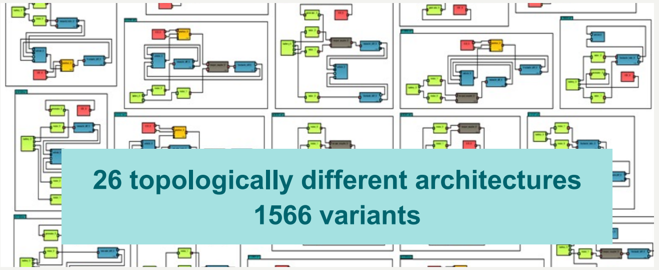
Global structure preserved
Local structure lost

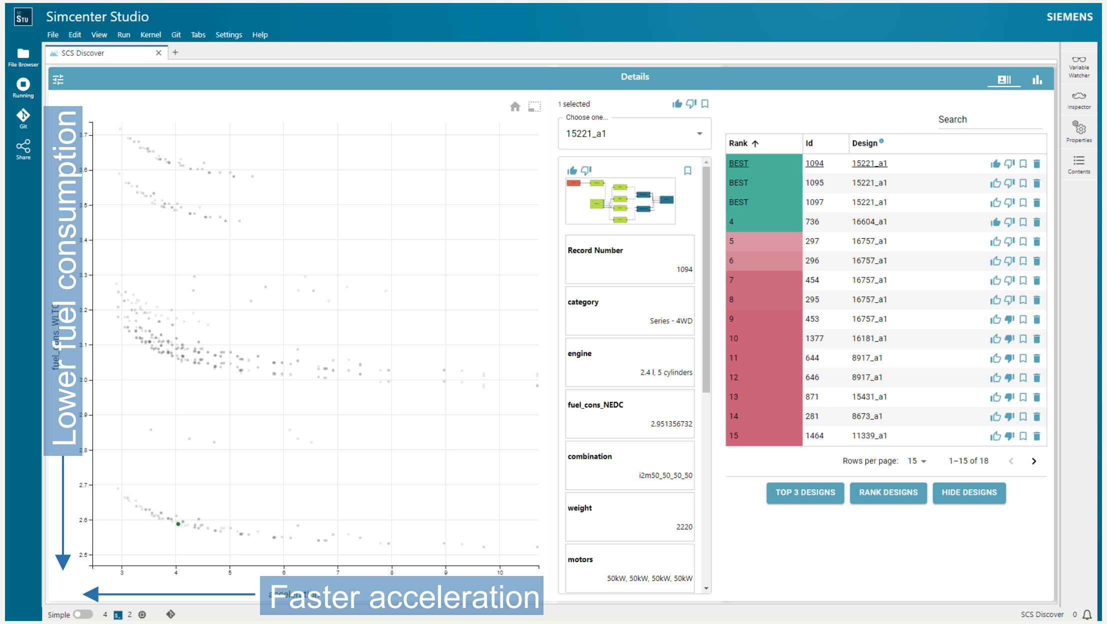




Use Case: HEV







Challenge

Design of the optimal hybrid powertrain combining including multiple combustion engine and electric motor variants

Solution

Use Simcenter Studio to generate and evaluate 100s of powertrain architecture alternatives

Benefit

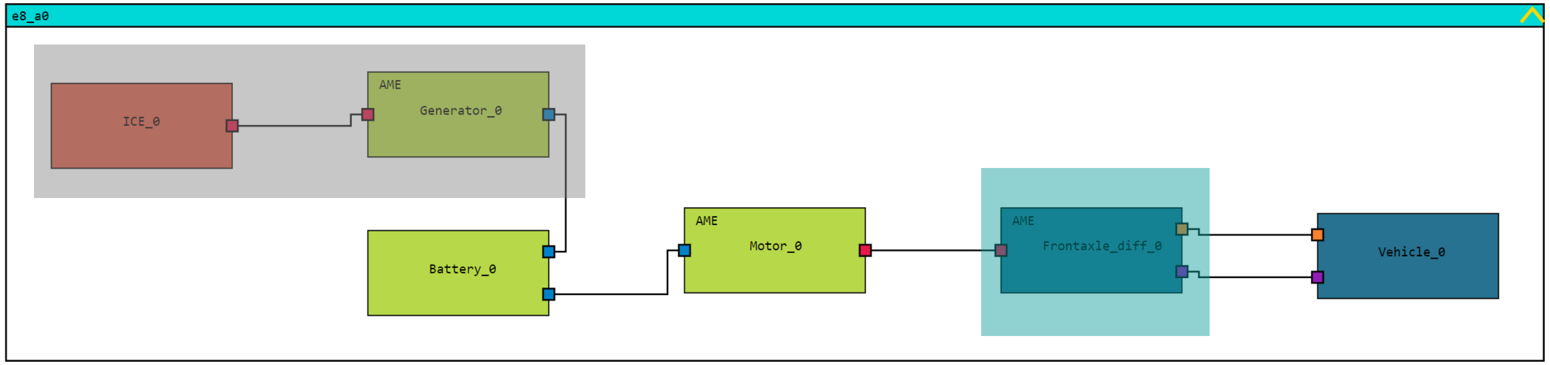
- Over 1500 powertrains generated and evaluated on multiple KPIs
- 20% improvement in fuel consumption, 7% cost improvement, 6% better acceleration

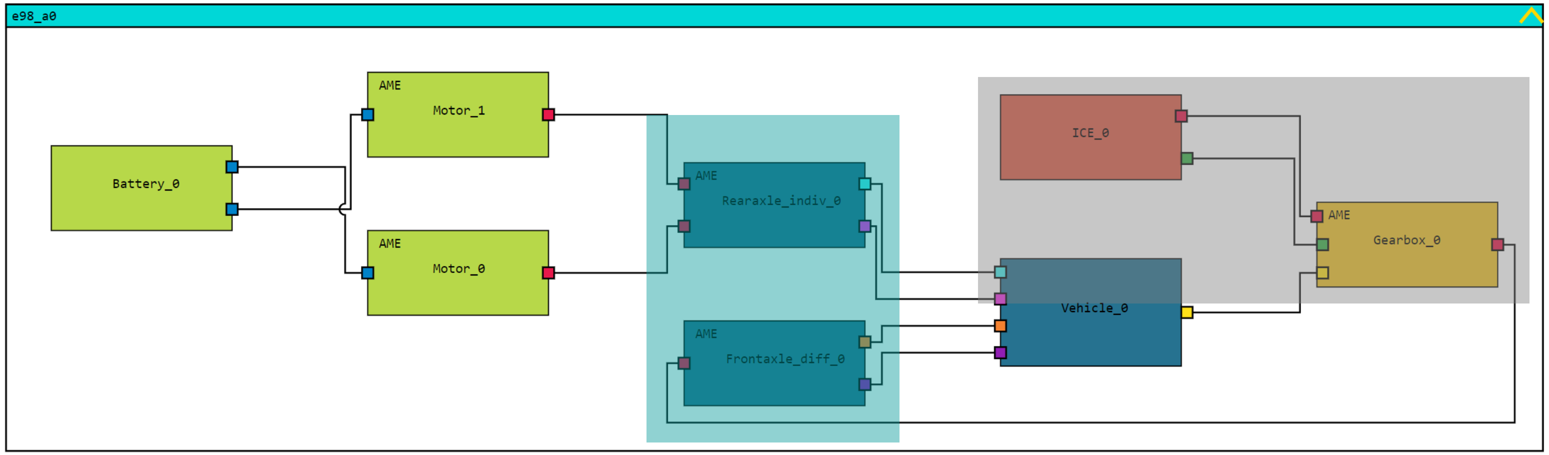
Vanhuyse J., Closed-loop Design Methodology for Hybrid Electric Vehicle Powertrains. 2018.

Use Case: HEV

Architectures

26 Architectures





Variants

1566 Variants

- ICE: 1, 2, 3
- Electric motor: 1, 2, 3
- # Electric motor: 1, …, 4
- # Torque coupler: 0, 1
- # Generator: 0, 1
- # Gearbox: 0, 1
- Axles: front, rear, or both

Use Case: HEV

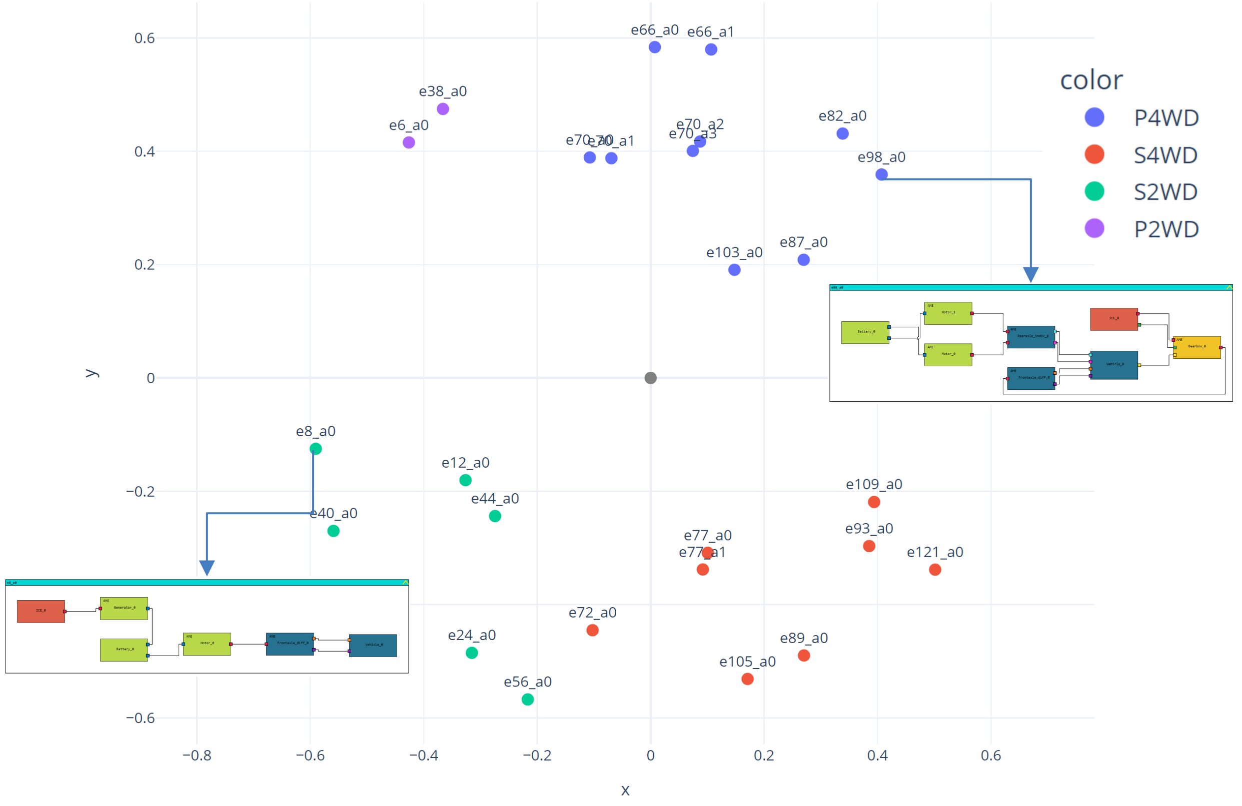
Architectures

X-axis for parallel / series
y = -0.15 for wheel drive

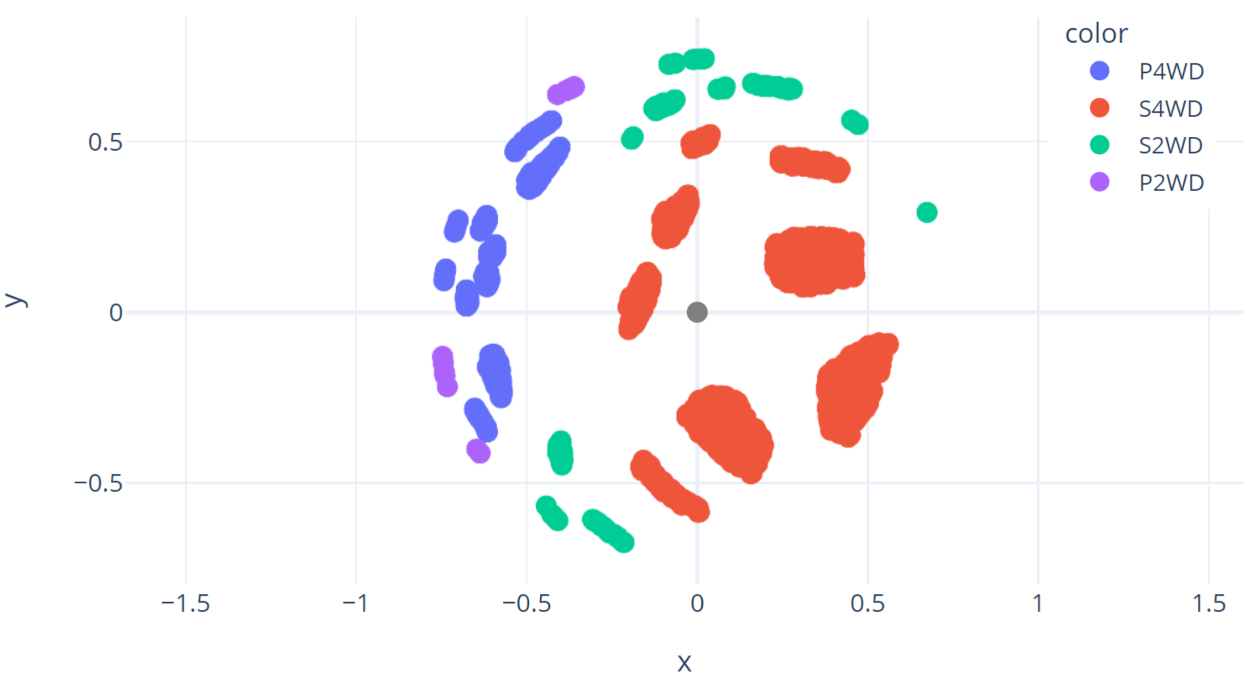
Variants

MDS fails
Computation time 104s

HEV architectures coordinates - MDS



HEV variants coordinates - MDS



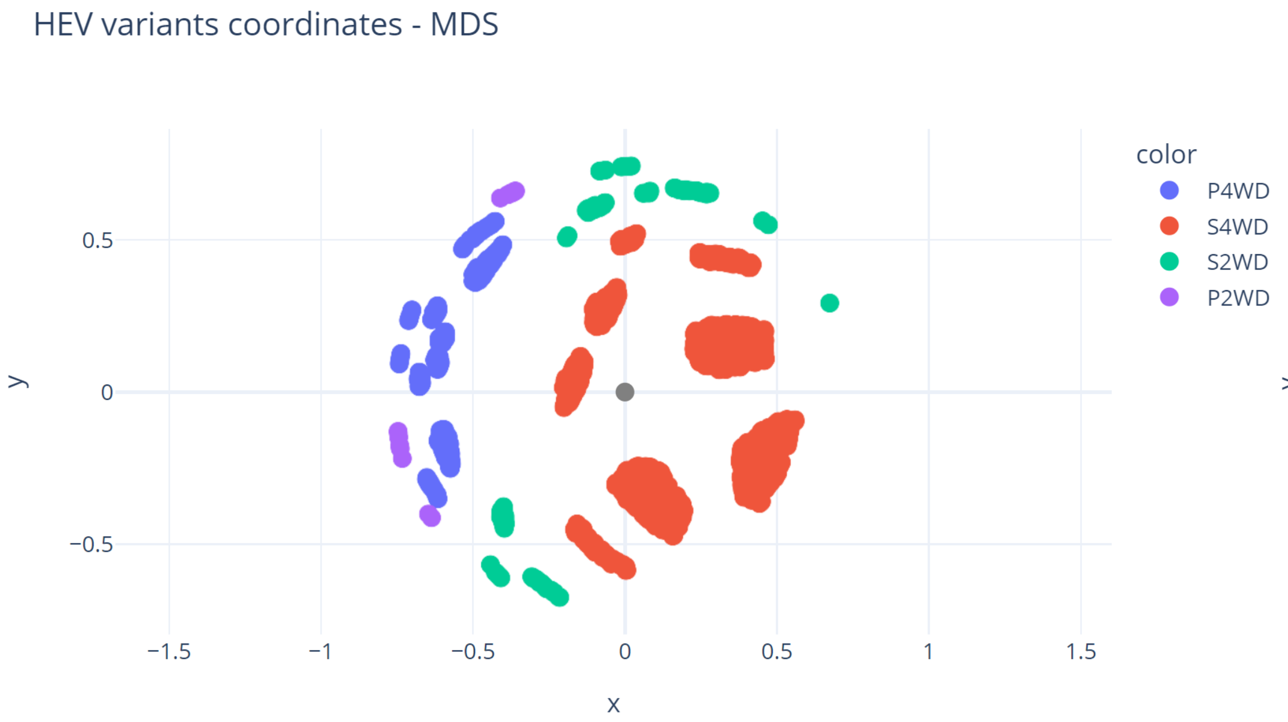
Use Case: HEV – DR Comparison

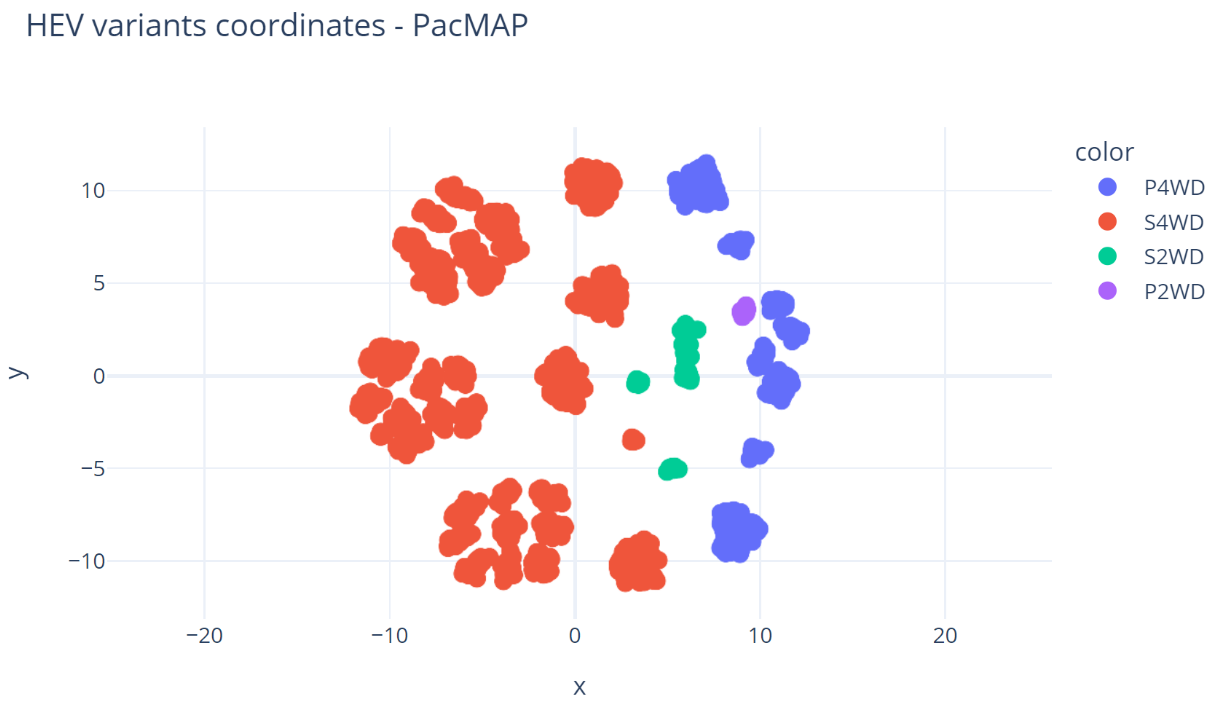
Variants

MDS fails
Computation time 104s

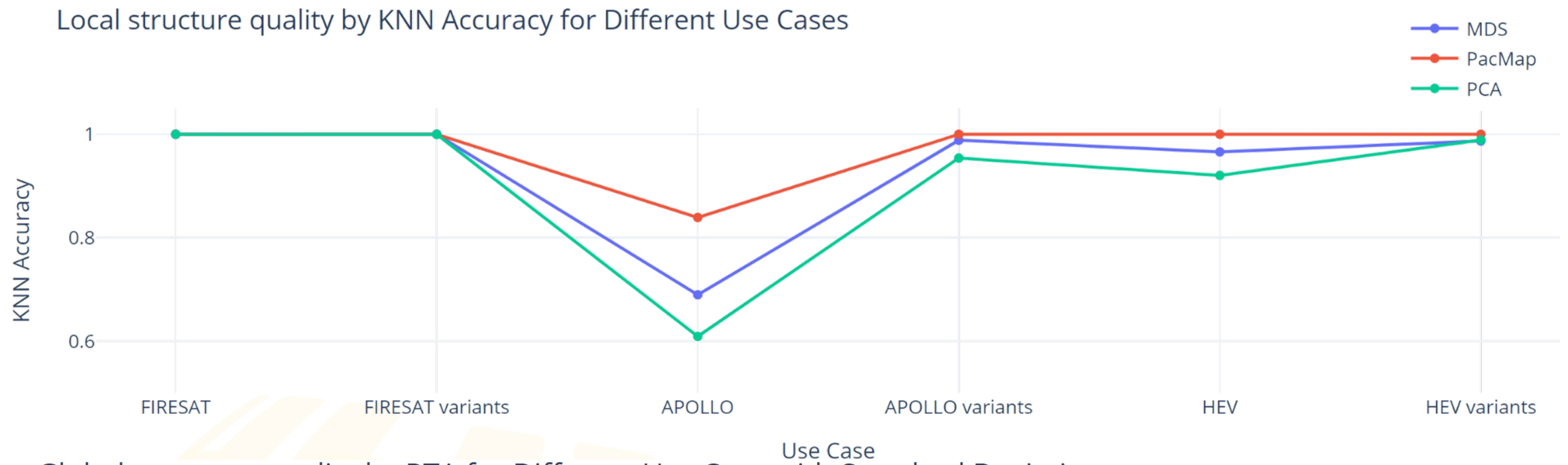
Variants

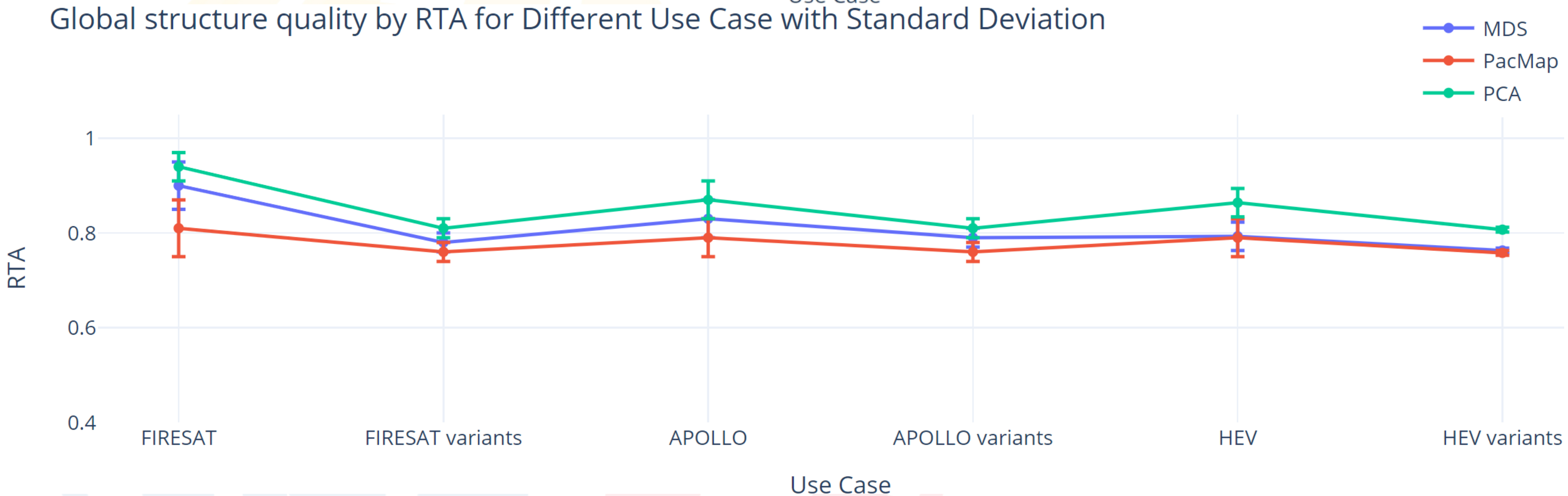
PacMAP preserves clusters
Computation time 10s



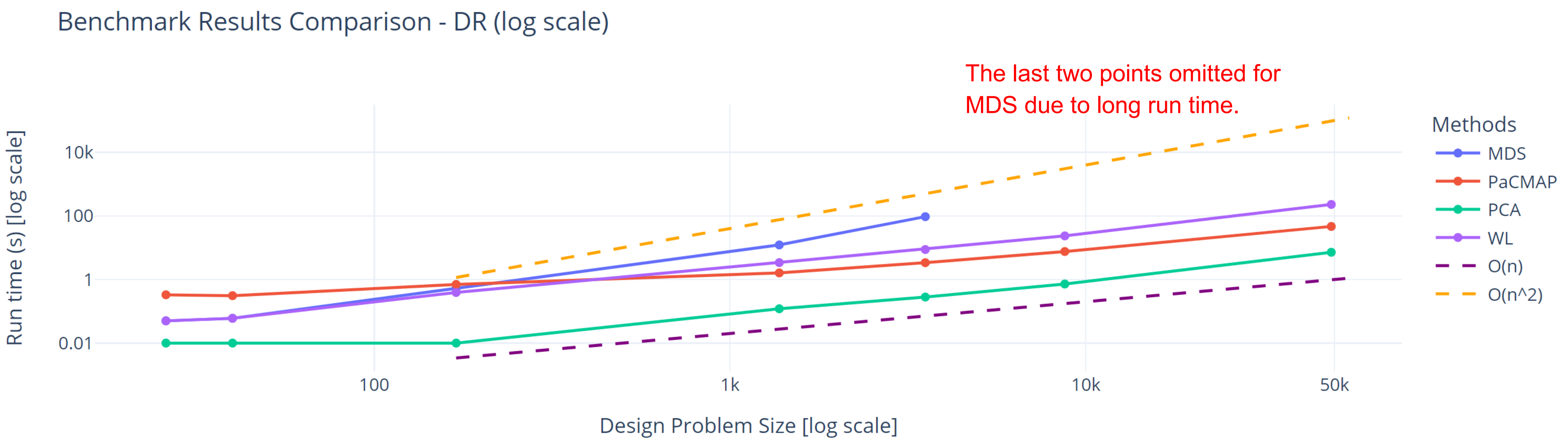


Quantitative Evaluation Results



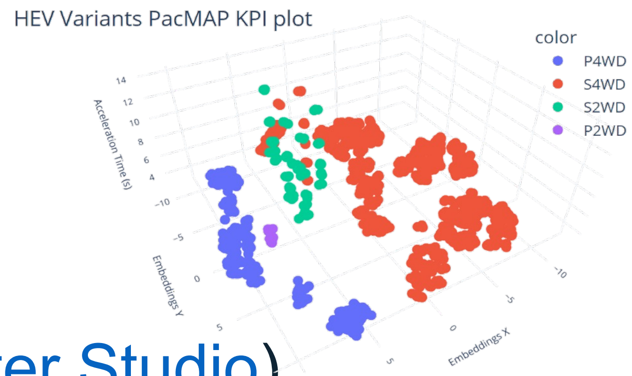


Quantitative Evaluation Results



Method	Year	Type	Structure	Speed	Precision	Tuning
MDS	1964	Exact	Both	Slow	High	No
PaCMAP	2021	Approximate	Local	Medium	Medium	Yes
PCA	1901	Projection	Global	Fast	Low	No

Conclusion



Conclusion

- **Generative methods** available for engineering ([Simcenter Studio]())
- **Challenges** in data interpretation
- **Machine Learning** solutions for navigating complex trade space
- **Similarity & dissimilarity** of topologically different, unlabeled designs
- **Real-world engineering problems** from automotive, aerospace, and defense

Q&A

Thank you for your attention! Any questions?

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34th Annual INCOSE international symposium

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July 2 - 6, 2024

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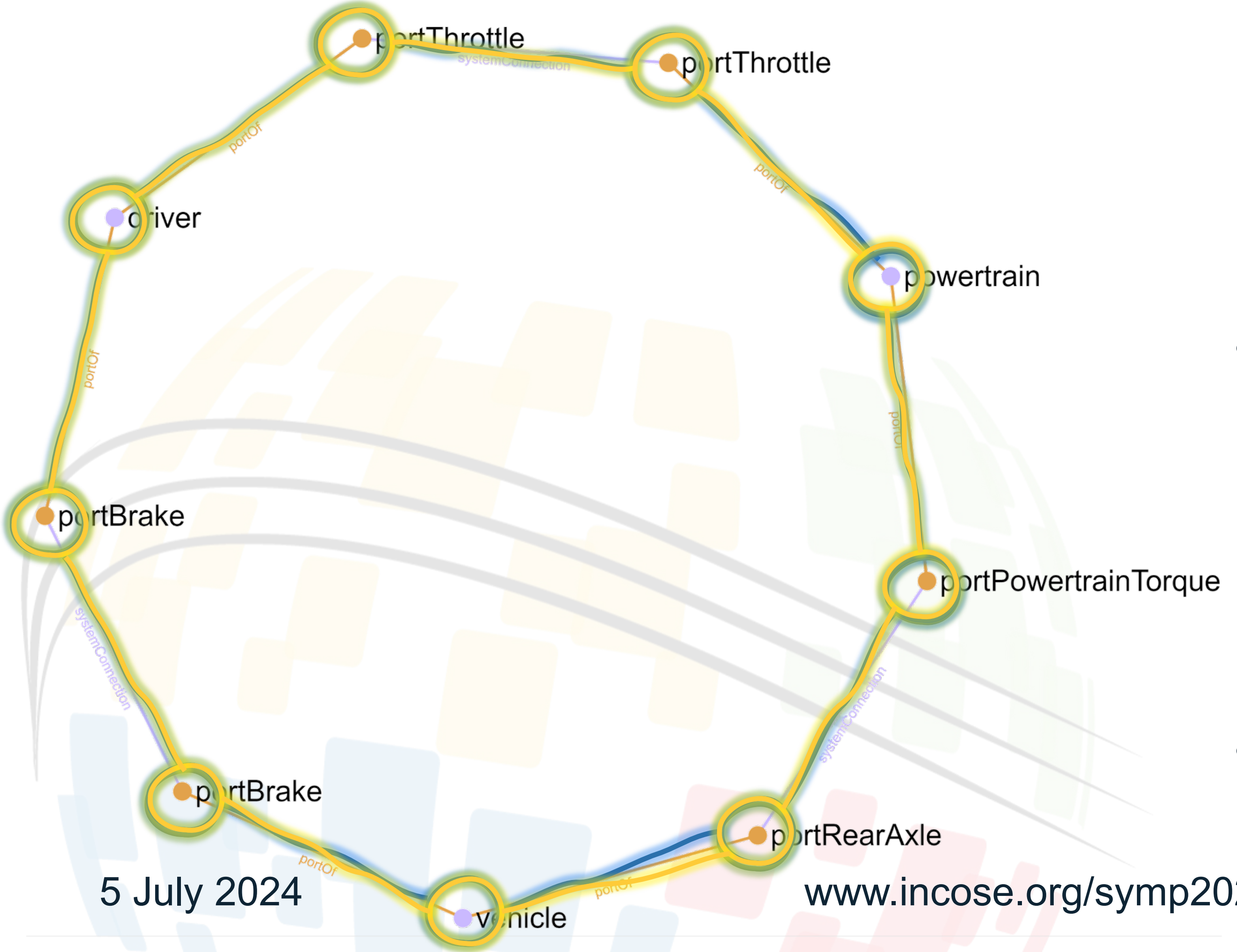
Back Up Slides

Graph Embeddings

Graphs

Components and ports as nodes
Relationships as edges
Parameters as node attributes



Embeddings

Iterative counting:

- Initialization, [driver, powertrain, vehicle, portBrake, …]
- It=1, [driver_portBrake _portThrottle, portThrottle_driver_portThrottle, ...]
- It=2, [driver_portBrake _portThrottle_portBrake_portThrottle, ...]
- And so on...

Benchmark creation

- Add more variabilities
- Relax the constraints