TECHNISCHE UNIVERSITÄT WIEN

CAIML Center for Artificial Intelligence and Machine Learning

3rd CAIML Symposium

“What’s next?”

FREQUENTIS

mc•p ALGORITHM FACTORY

PALFINGER

IMMO UNITED
Ihre Grundbuchexperten

10:30	Welcome Addresses by **Jasmin Gründling-Riener** (*Vice Rector Academic Affairs*) **Georg Sedlbauer** (*Federal Ministry for Climate Action, Environment, Energy, Mobility, Innovation and Technology - BMK*) Presentation of **iCAIML Doctoral College**
12:00	Lunch Break & Networking
13:00	Scientific Talks / Luc de Raedt and Martina Seidl
15:30	Coffee Break
16:00	Panel Discussion
17:00	Networking

TECHNISCHE UNIVERSITÄT WIEN

Center for Artificial Intelligence and Machine Learning

iCAIML DOCTORAL COLLEGE

"Innovative Combinations and Applications of AI and ML"

https://caiml.org/icaiml/

FREQUENTIS

ALGORITHM FACTORY

The mission of our doctoral college on “Innovative Combinations and Applications of AI and ML” is to investigate the combination of symbolic- and sub-symbolic AI techniques in connection with novel application domains.

Goals:

- Provide top research training committed to excellence in the field of AI and ML, with a unique combination of the areas of symbolic and sub-symbolic AI
- Educate doctoral students to address complex research problems in connection with concrete application domains
- Establish sustainable know-how exchange in the field of symbolic AI and ML through a tight collaboration between industrial and university partners with a focus on foundational problems
- Making the next generation of AI researchers aware of the impact (ethical, environment, etc.) their work might have and define concrete for measures for doing so (in connection with the Digital Humanism activities of TU Wien)

We expect synergetic effects in both directions:

(1) novel combinations of AI methods can pave the way for applications of AI techniques in so far less explored domains

(2) the requirement in specific applications can guide and instruct fundamental research in the field of AI.

This calls for collaboration

- Between different faculties of TU Wien
- With industry partners

Following faculties are part of iCAIML

- Faculty of Informatics
- Faculty of Mathematics and Geoinformation
- Faculty of Architecture and Planning
- Faculty of Physics
- Faculty of Technical Chemistry

iCAIML head and deputy

Stefan Woltran

Sabine Andergassen

iCAIML supervisors 1/2

Sabine Andergassen

Ivona Brandic

Agata Ciabattoni

Thomas Eiter

Peter Filzmoser

Thomas Gärtner

Clemens Heitzinger

Martin Kampel

iCAIML supervisors 2/2

Peter Knees

Georg Madsen

Nysret Musliu

Julia Neidhardt

Emanuel Sallinger

Stefan Szeider

Milica Vujovic

Stefan Woltran

iCAIML 16 projects

- Graph Neural Networks
- Reinforcement Learning for Enhancing Sepsis Treatment
- Towards Explainable and Knowledge-driven Large Language Models
- Mathematical Methods in AI
- Decision Support in Air-Traffic Control
- Advanced Solving Techniques for Production Planning and Scheduling
- Logical Methods for Deontic Explanations in Law
- Developing Declarative ASP Models with Interactive LLM use
- AI for Dementia Care
- Declarative and Hybrid AI in Financial Knowledge Graphs
- Integrating Large Language Models in Automated Constraint Programming Optimization
- AI-supported Higher Education Learning Spaces: AI-Enabled Teaching Strategy Optimization
- Supporting Senior Long-term Care Environment Design through Knowledge Graph-Driven Architectural Design
- Atomistic Simulations of Electrochemical Interfaces
- Microscopic Derivation of Effective Lattice Model Hamiltonians for Long-Range Interacting Atoms
- AI for Communication in Hybrid Classic Quantum Systems

iCAIML 16 projects

- **Graph Neural Networks**
- **Reinforcement Learning for Enhancing Sepsis Treatment**
- **Towards Explainable and Knowledge-driven Large Language Models**
- Mathematical Methods in AI
- Decision Support in Air-Traffic Control
- Advanced Solving Techniques for Production Planning and Scheduling
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- Microscopic derivation of effective lattice model Hamiltonians for long-range interacting atoms
- **AI for Communication in Hybrid Classic Quantum Systems**

Reinforcement Learning for Enhancing Sepsis Treatment

Supervisor: Clemens Heitzinger

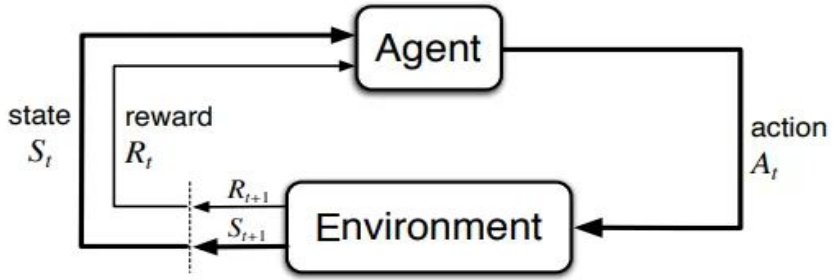
Researcher: Mohammad Mahdi Azarbeik

Objectives:

Developing a reinforcement learning algorithm to optimize corticosteroid therapy in sepsis, leveraging high-resolution clinical data from intensive care databases to enhance treatment decision-making and decrease sepsis-related mortality.

Methodology: Leveraging Reinforcement Learning

- Utilizing High-Resolution Clinical Data (MIMIC, AmsterdamUMCdb, and AKH database)
- Modeling Patient Environment with MDP, defined by the tuple {S,A,T(s',s,a),R(s'),γ}
- Terminal states: A positive reward for survival and a negative penalty for death.

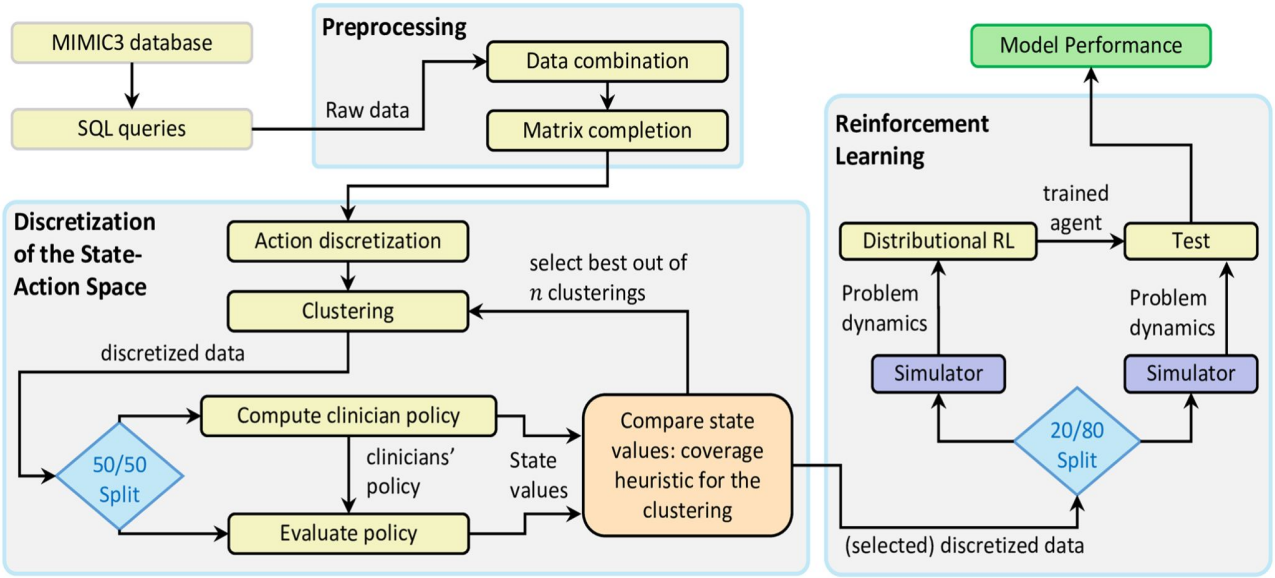


Experiments

- Clustering time series data
- Off-Policy Deep Distributional RL
- HCOPE

Expected Results:

- Decreased Sepsis-Related Mortality



Overall flowchart of the experiments. [2]

Further reads:

- [1] Bologheanu, R., Kapral, L., Laxar, D., et al. Development of a Reinforcement Learning Algorithm to Optimize Corticosteroid Therapy in Critically Ill Patients with Sepsis. J. Clin. Med. 2023, 12, 1513. https://doi.org/10.3390/jcm12041513
- [2] Böck M, Malle J, Pasterk D, Kukina H, Hasani R, et al. (2022) Superhuman performance on sepsis MIMIC-III data by distributional reinforcement learning. PLOS ONE 17(11): e0275358. https://doi.org/10.1371/journal.pone.0275358
- [3] Komorowski, M., Celi, L.A., Badawi, O. *et al.* The Artificial Intelligence Clinician learns optimal treatment strategies for sepsis in intensive care. *Nat Med* 24, 1716–1720 (2018). https://doi.org/10.1038/s41591-018-0213-5

AI for Communication in Hybrid Classic Quantum Systems




Supervisors: Ivona Brandic, Vincenzo De Maio

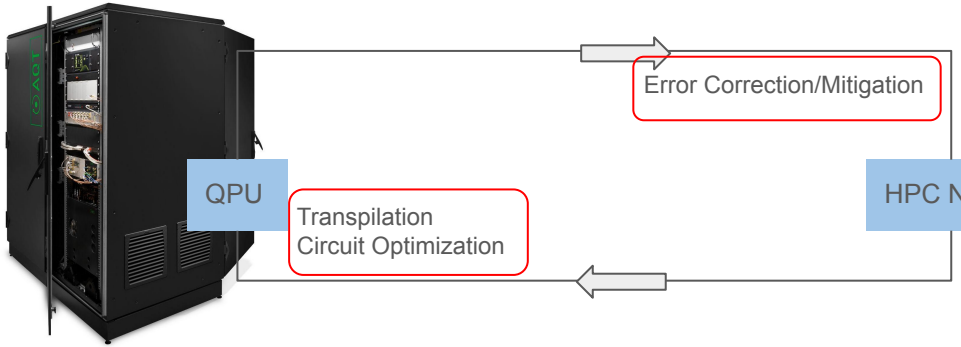
Researcher: Sabrina Herbst

Co-supervision: Sabine Andergassen

Objectives:

The goal of this project is to use ML techniques for the integration of hybrid systems in the Post-Moore era.

High-Performance integrated Quantum Computing



Publications:

- **Herbst, S** et al. 2024. Streaming IoT Data and the Quantum Edge: A Classic/Quantum Machine Learning Use Case. In: Zeinalipour, D., *et al.* Euro-Par 2023: Parallel Processing Workshops. Euro-Par 2023. Lecture Notes in Computer Science, vol 14351. Springer, Cham
- De Maio, V. et al. 2022. A Roadmap To Post-Moore Era for Distributed Systems. In Proceedings of the 2022 Workshop on Advanced tools, programming languages, and PLatforms for Implementing and Evaluating algorithms for Distributed systems (ApPLIED '22). Association for Computing Machinery, New York, NY, USA, 30–34.
- De Maio, V. et al. 2024. Training Computer Scientists for the Challenges of Hybrid Quantum-Classical Computing. To appear at CCGRID 2024.

Quantum Machine Learning

Promising field

- Speed-Ups
- Space-Efficiency
- Expressivity

Quantum Information Theory provides an alternative way of thinking

- How can we process information more efficiently?
- How can quantum phenomena be exploited to lead to advantages?

⟹ New paradigms: **Quantum-Inspired Machine Learning**

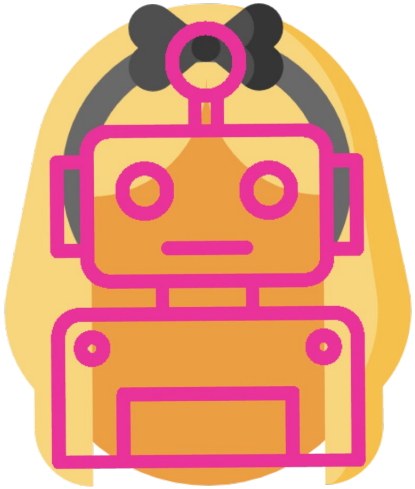
Declarative and Hybrid AI in Financial Knowledge Graphs

Supervisor: Emanuel Sallinger

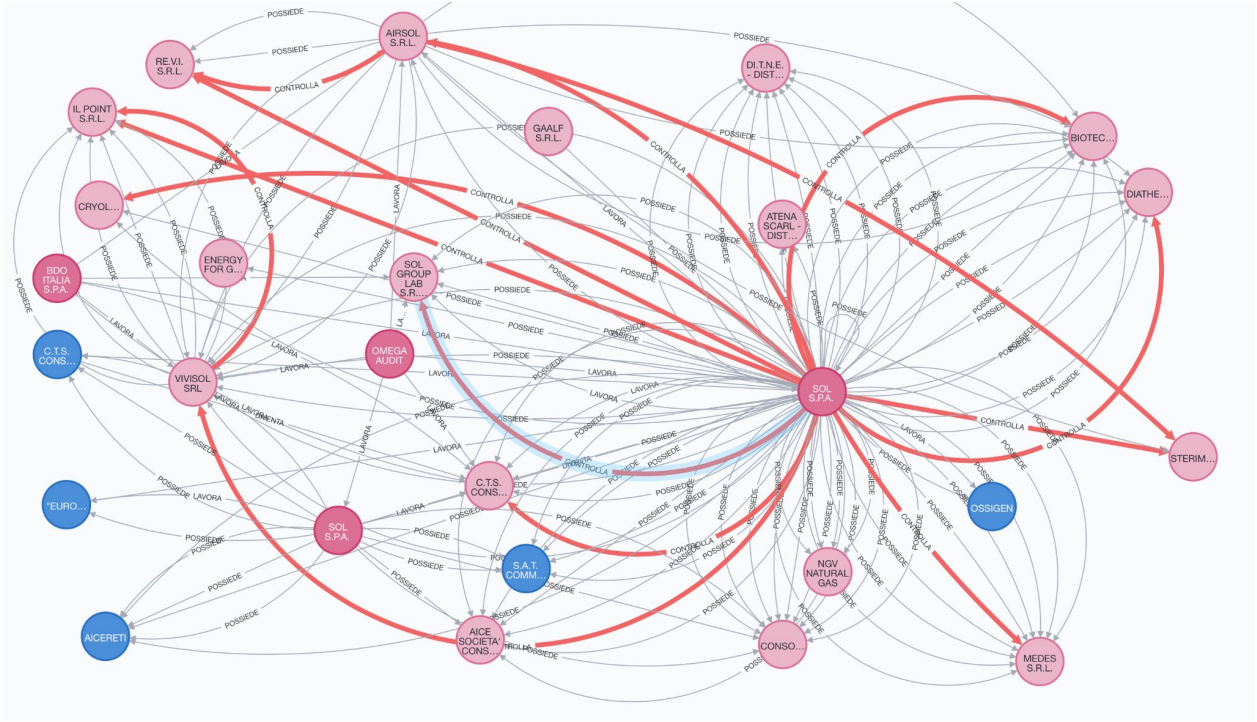
Researcher: Livia Blasi

Objectives:

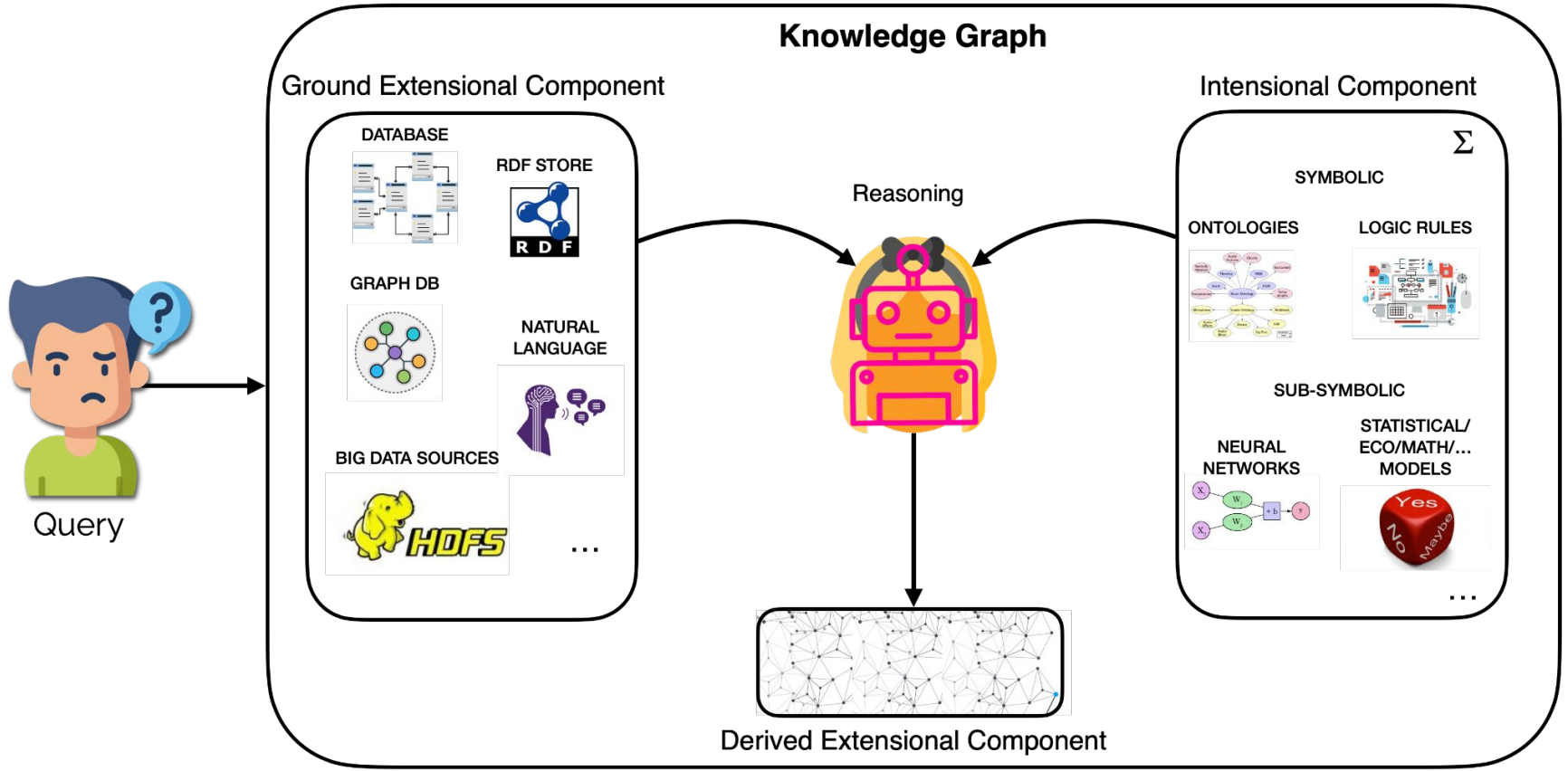
On the side of declarative AI, our objective is to develop logical reasoners based on Vadalog that are able to handle such temporal, financial Knowledge Graphs as well as the scale of data encountered here. On the side of hybrid AI, we aim to include Knowledge Graph embeddings (KGEs), Graph Neural Networks (GNNs) and/or Large Language Models (LLMs), as required by the specific research questions.



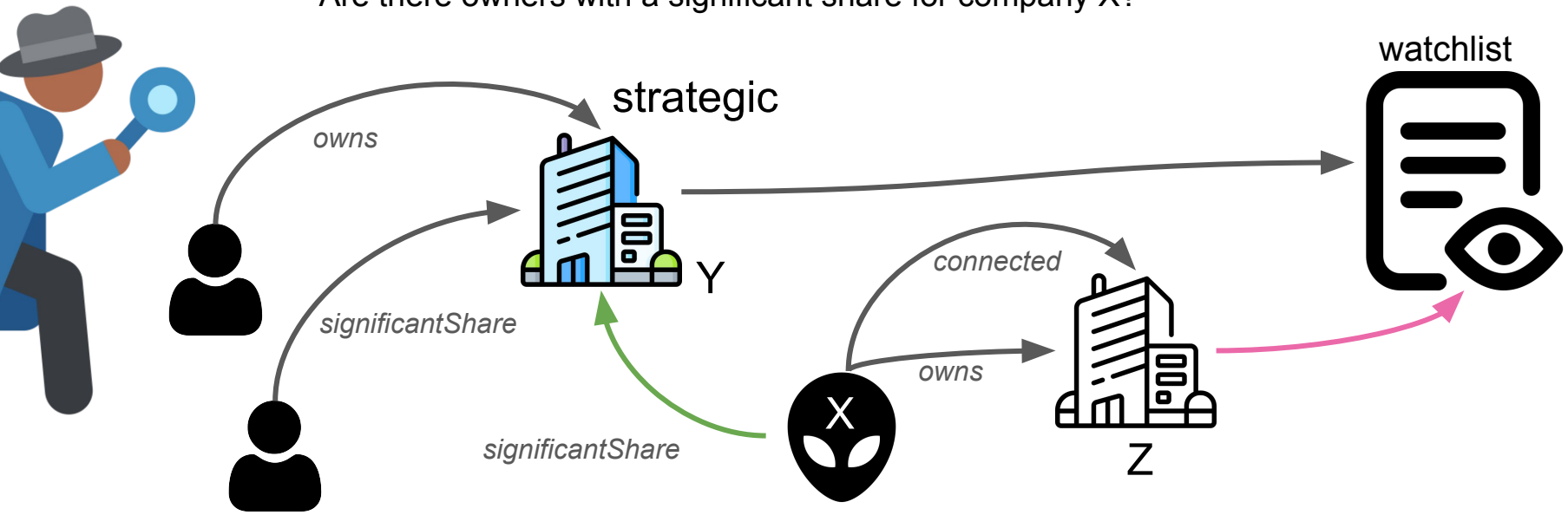
Italian Companies KG



Intensional knowledge + Extensional knowledge


Knowledge Graph
Ground Extensional Component
DATABASE
RDF STORE
R D F
GRAPH DB
NATURAL LANGUAGE
BIG DATA SOURCES
HDFS
...
Reasoning
Intensional Component
Σ
SYMBOLIC
ONTOLOGIES
LOGIC RULES
SUB-SYMBOLIC
NEURAL NETWORKS
STATISTICAL/ ECO/MATH/... MODELS
Yes
No
Maybe
...
Query
Derived Extensional Component

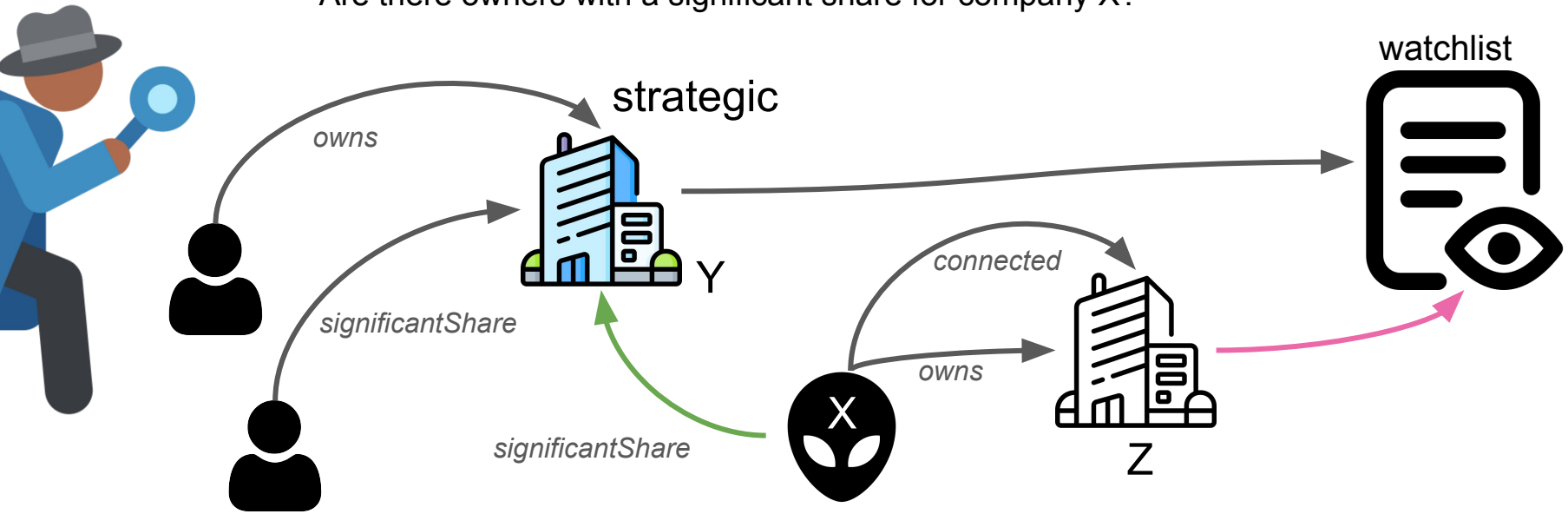
Are there owners with a significant share for company X?



$$significantShare(X, Y) \rightarrow significantOwner(X, Y)$$

$$watchCompany(Y), significantOwner(X, Y), connected(X, Z) \rightarrow watchCompany(Z)$$

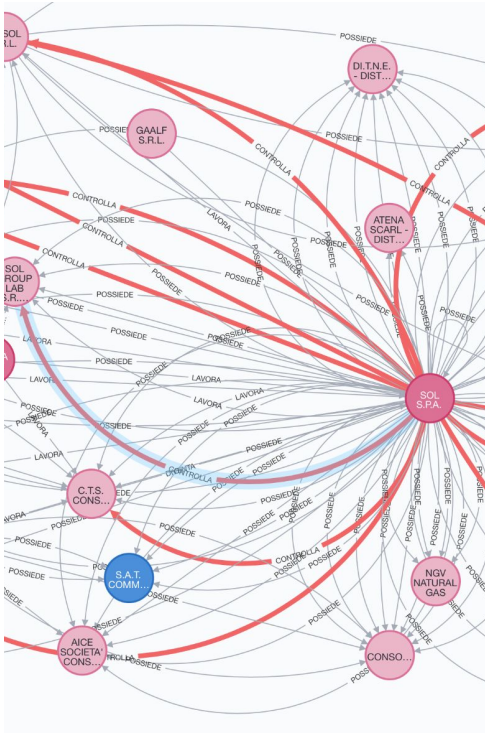
Are there owners with a significant share for company X?



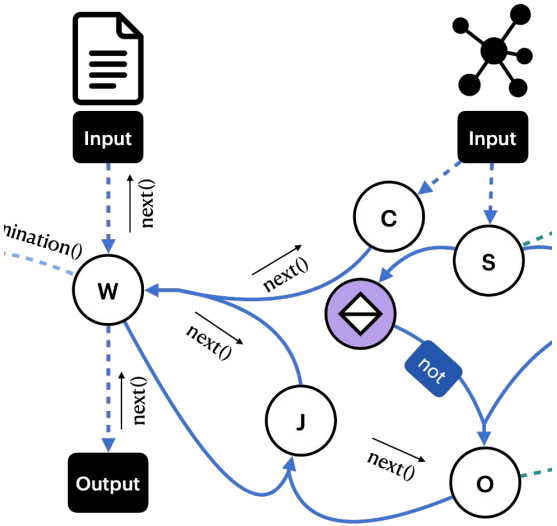
$$\boxminus_{[0,1]}\, significantShare(X,Y), \neg \diamondminus_{(1,2]}\, significantShare(X,Y) \rightarrow significantOwner(X,Y)$$

$$watchCompany(Y), significantOwner(X,Y), connected(X,Z) \rightarrow watchCompany(Z)$$

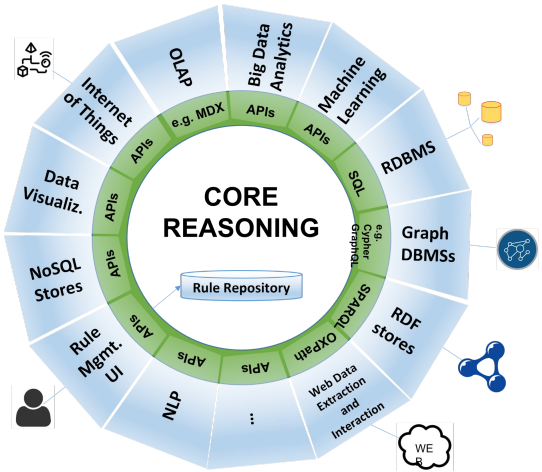
Building Knowledge Graphs



Designing AI Algorithms



Building AI Systems (Temporal Vadalog)



Towards Explainable and Knowledge-driven LLMs



Stefan Woltran, Peter Knees

researcher: Ilya Lasy

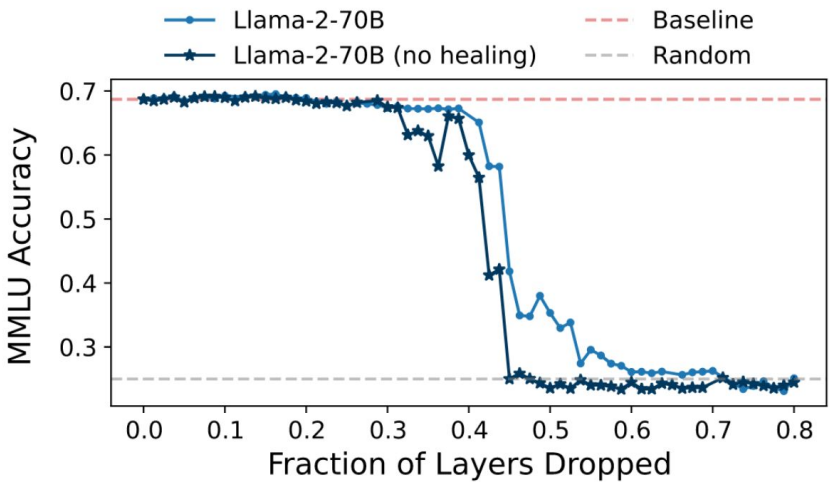
Objectives:

The goal of the thesis is to investigate the inner workings of Large Language Models and other domain-specific Transformer-based architectures to gain a deep understanding of the learned representations and inference processes. This understanding shall then serve as foundation to build interpretable systems based on explicit knowledge, in particular with the goal to guarantee outputs of a certain quality and avoid so-called “hallucinations”.

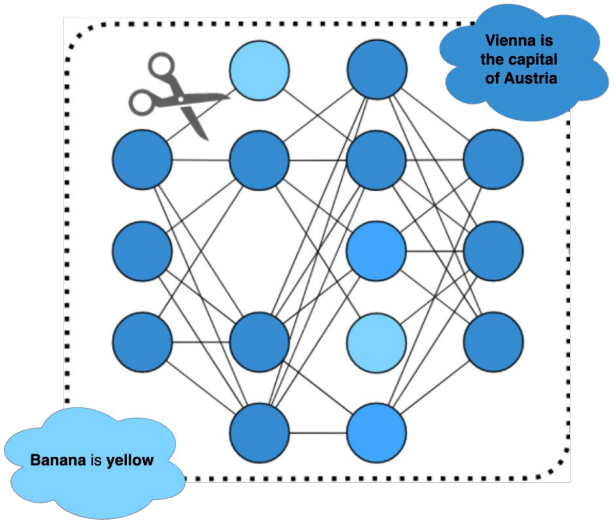
LLM flaws:

- *End-to-end (single module)*
- *Overparameterized (Contains non-informative weights)*
- *Requires domain specific fine-tuning*
- *No clear understanding on **what**, **where** and **how** knowledge is stored*

(Gromov et.al 2024)



(Bayazit et.al 2023)

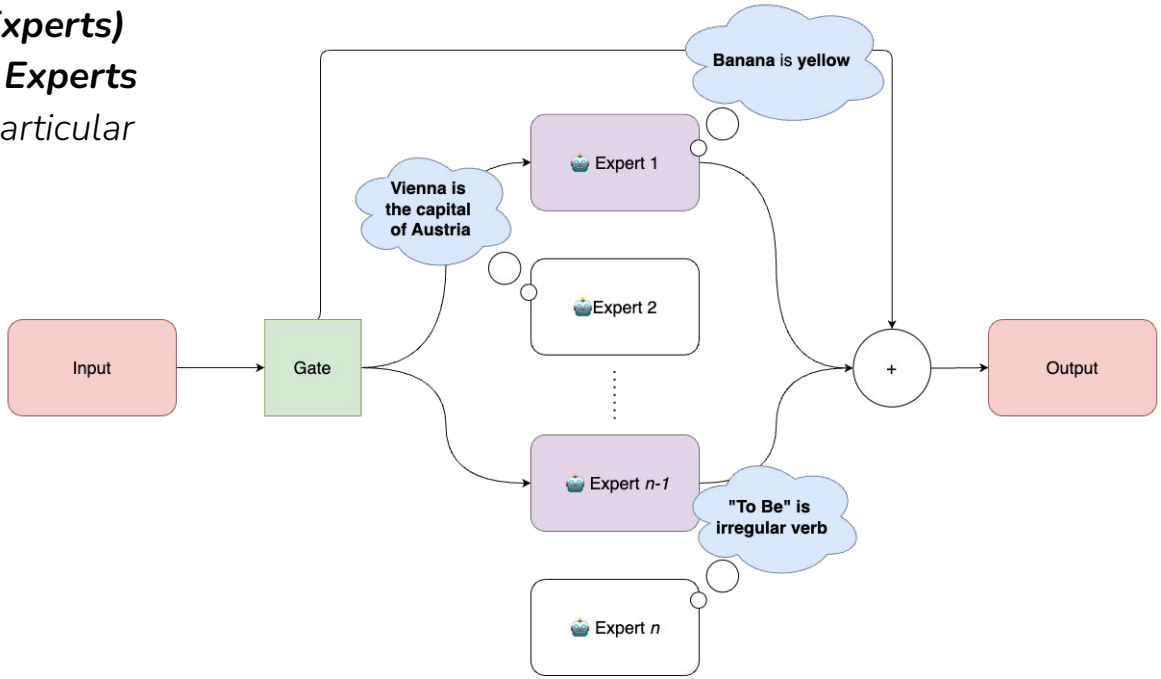


Proposal: *make LLM interpretable and efficient* ***by design (Mixture Of Experts)***

- *LLM layers are splitted into* ***Experts***
- *Each expert specializes in particular* ***knowledge type***

Knowledge:

- *World Facts*
- *Commonsense knowledge*
- *Linguistic*
- *Task/Domain Specific*
- *...*



Integrating LLMs in Automated Constraint Programming Optimization



Stefan Szeider, Julia Neidhardt

researcher: Florentina Voboril

Objectives:

The main objective of this project is to combine the power of Large Language Models (LLMs) for automated Constraint Programming (CP) optimization. More specifically, the plan is to use LLMs to come up with streamlining constraints, implied (redundant) constraints, symmetry-breaking constraints, and dominance-breaking constraints.

Constraint Programming

- Programming paradigm
- Relationships between variables
- Solver

```
% Constraints to ensure all numbers in each row and column are different
constraint forall (c in COLS) (alldifferent([Latin_square[r,c] | r in ROWS]));
constraint forall (r in ROWS) (alldifferent([Latin_square[r,c] | c in COLS]));
```

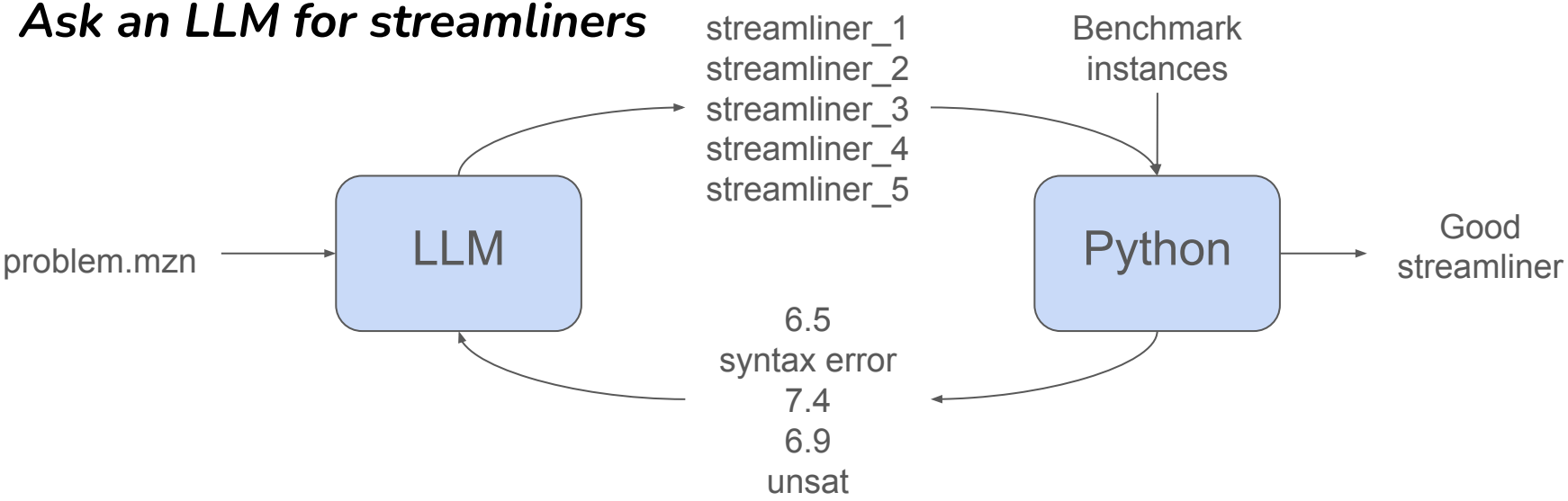
Example: Latin Square

Streamliners

- Additional constraints
- Focus on promising segments of the search space

```
% Streamliner: Fixing Diagonal Values
constraint forall(i in 1..n) (Latin_square[i,i] = i);
```

Ask an LLM for streamliners



- Can LLM streamliners compete with streamliners suggested by human experts?
- How to give feedback to the LLM for improved streamliners?
- Are LLMs capable of mathematical reasoning (and not just plagiarize answers they have been trained with)?
- Can we find LLM streamliners in a real-time setting competitively?

Graph Neural Networks



Thomas Gärtner, Stefan Szeider

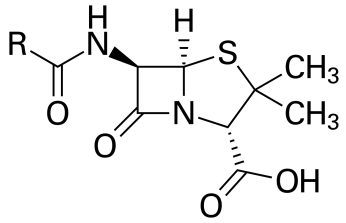
researcher: Fabian Jogl

Objectives:

The objective of our research is

1. to improve the understanding of what functions graph neural networks can express
2. to develop graph neural networks that can express more functions.

What is a GNN?

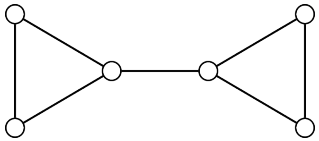


GNN

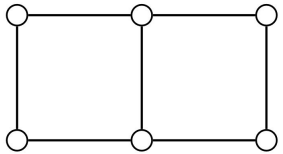
Antibiotic?

(Cell 2020)

GNNs are not sufficiently expressive:



GNN



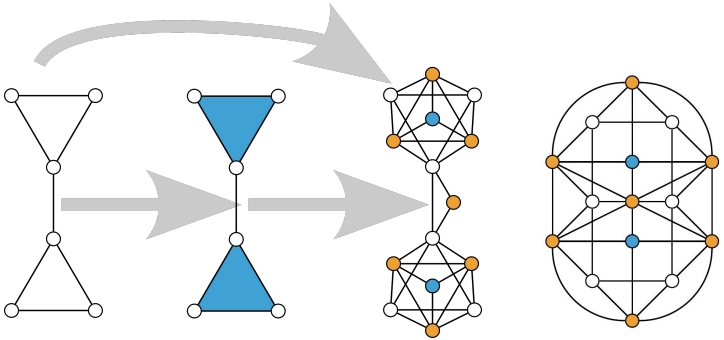
GNN

Identical Predictions

(Xu et al. 2019, Morris et al. 2019)

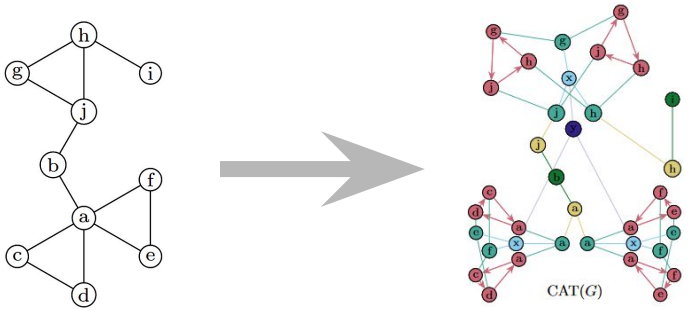
Expressivity as graph transformation:

(NeurIPS 2023)



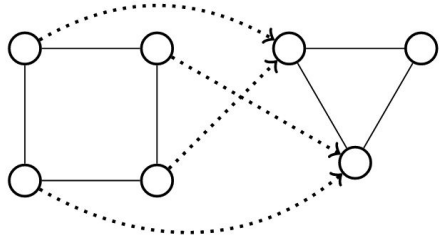
Maximal expressivity for outerplanar graphs:

(GLF@NeurIPS 2023)



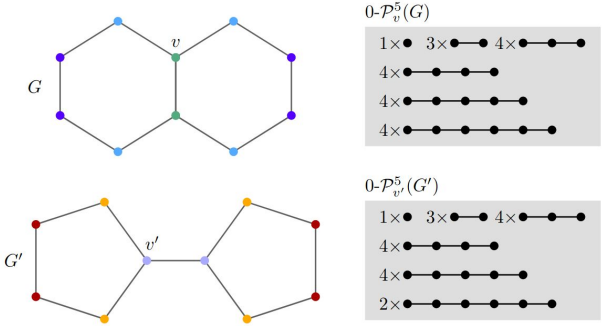
Sampling Homomorphism Improves GNNs

(ICML 2023)



Path Information Improves GNNs

(ICML 2024)



iCAIML ecosystem

CoE MECS (Materials for Energy Conversion and Storage)

MECS – Cluster of Excellence
MATERIALS FOR ENERGY CONVERSION AND STORAGE

MSCA COFUND LOGICS

MSCA COFUND ENROL - Engineering for Life Sciences

Doctoral College on Digital Humanism

Innovative Combinations and Applications of AI and ML

Informatics Doctoral School

Cluster of Excellence

Bilateral AI

FREQUENTIS
FOR A SAFER WORLD

Specialist for communication and information solutions for safety-critical control centres

Georg Trausmuth
Director Corporate Research

We set standards in control centres worldwide

FREQUENTIS

Global specialist driven by know-how, experience, and synergies

Professional services

- Voice and data communications
- Cyber security: no safety without security
- Networking for safety-critical communications and information
- Drone detection, management, and interception
- Situational awareness
- Digital tower solutions: classic and remote
- Actionable information management
- Surveillance
- ATM automation systems
- Synchronised traffic operations
- Incident and crisis management
- Mission-critical services

Common products and solutions

Innovation management

R&D: leveraging cross-industry heritage in product development

Frequentis group at a glance

30+ years of profitable growth

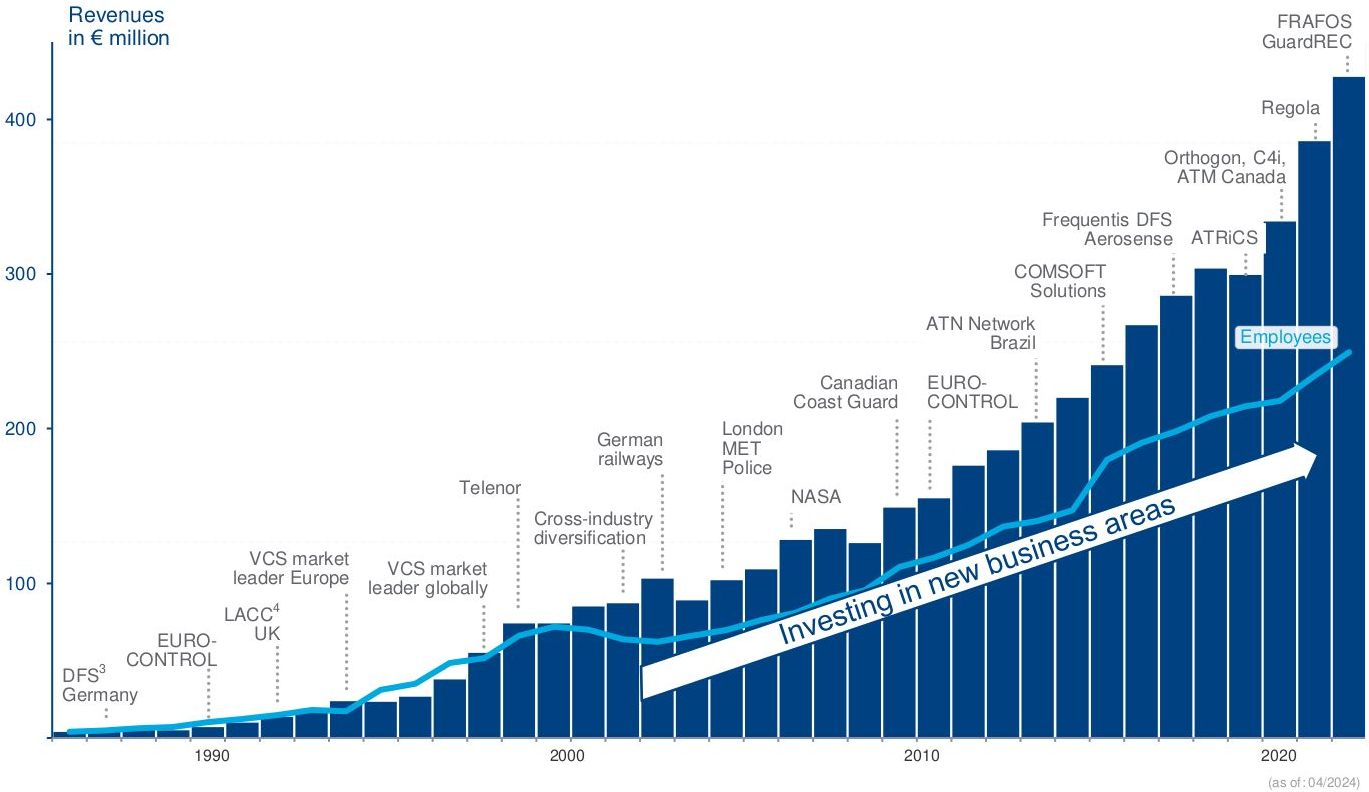
Established **1947**
Headquarters Vienna, Austria

75+
years experience with safety-critical applications

2,217
Employees[1]

75% STEM[2] & specialists
50+ nations

€427.5m
Revenues in 2023



(as of: 04/2024)

1) As of 2022: average in full-time equivalents (FTE); 2) Science, Technology, Engineering, Math 3) Deutsche Flugsicherung 4) London Area Control Centre, operated by NATS

A strong network around the world

500+ customers

150 countries

>90% of our customers are government agencies

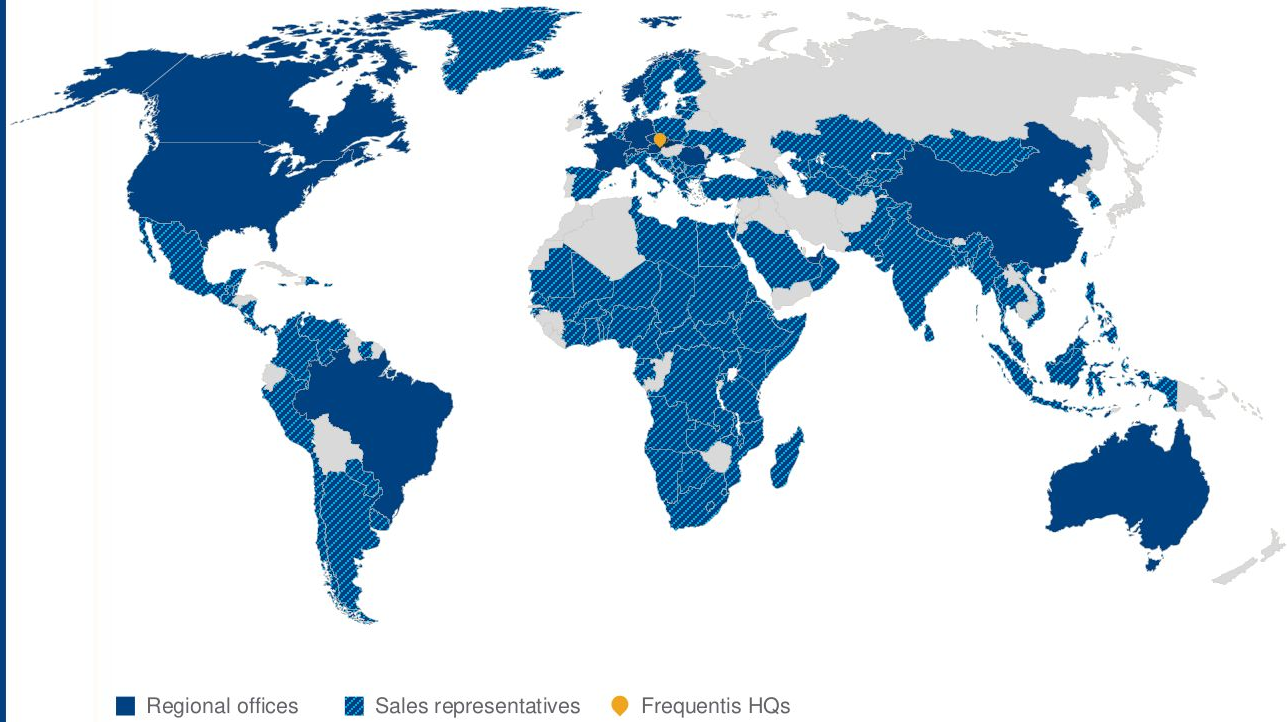
49,000+ working positions using Frequentis solutions

33% of the world safer with Frequentis networks

95% of all air traffic is safely managed by our technology

#1 in GSM-R dispatcher terminals

240,000 km largest maritime coastline protected



FREQUENTIS

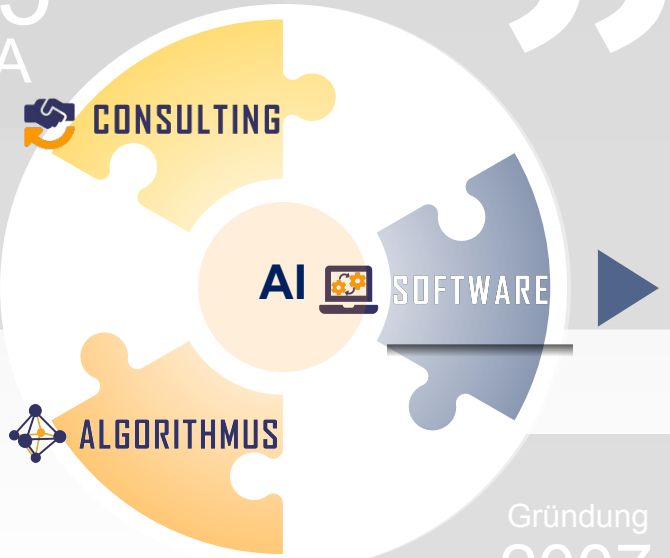
FOR A SAFER WORLD

Ziel mit KI: neue Kombinationen von Einschränkungen lösen

Mögliche Themen: Scheduling, Personaleinsatzplanung, Tourenplanung, Energiemanagement

ALGORITHM FACTORY

25 MA



Gründung 2007

Christian Doppler Forschungsgesellschaft

Wir optimieren diese Planungsprozesse unserer Kunden:

Sales & Operations Planning — Demand & Supply

Advanced Planning & Scheduling
Opcenter APS — Grobplanung, Feinplanung

Workforce Management — Personaleinsatzplanung

Profitabilität | Prozessqualität | Transparenz | Kundenservice

- CAIML students seminar
- iCAIML retreat
- Digital Humanism Summer School September 2-6

Thank you!
Enjoy lunch

12:00	Lunch Break & Networking
13:00	Cluster presentation by Thomas Eiter
13:30	Scientific Talks / Luc de Raedt and Martina Seidl
15:30	Coffee Break
16:00	Panel Discussion
17:00	Networking

Bilateral AI Cluster

presentation by Thomas Eiter

Scientific Talk **Martina Seidl**

Scientific Talk **Luc de Raedt**

Panel Discussion

Kees van Berkel, Julia Neidhardt, Stefan Neumann, Emanuel Sallinger, Milica Vujovic

Moderation: Ivona Brandic

Thank you!
Till may 2025