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Fraunhofer Institute for Integrated Systems and Device Technology IISB

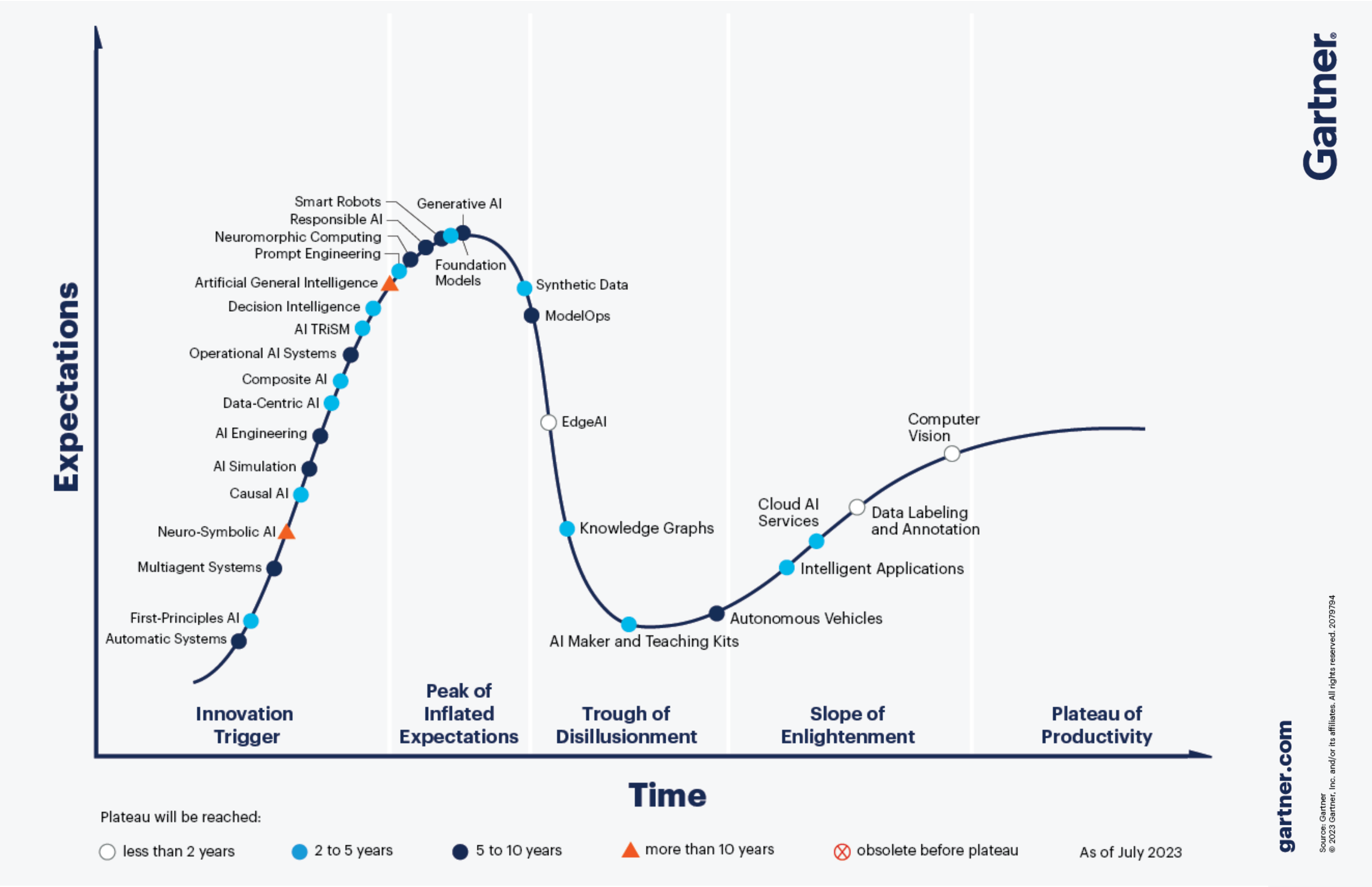
Physics and/or data science?
How AI will enhance simulation and engineering.

Dr. Andreas Rosskopf

IISB Annual Symposium 2023

October 12, 2023, Fraunhofer IISB, Erlangen, Germany

Hype Cycle for AI 2023 (by Gartner)



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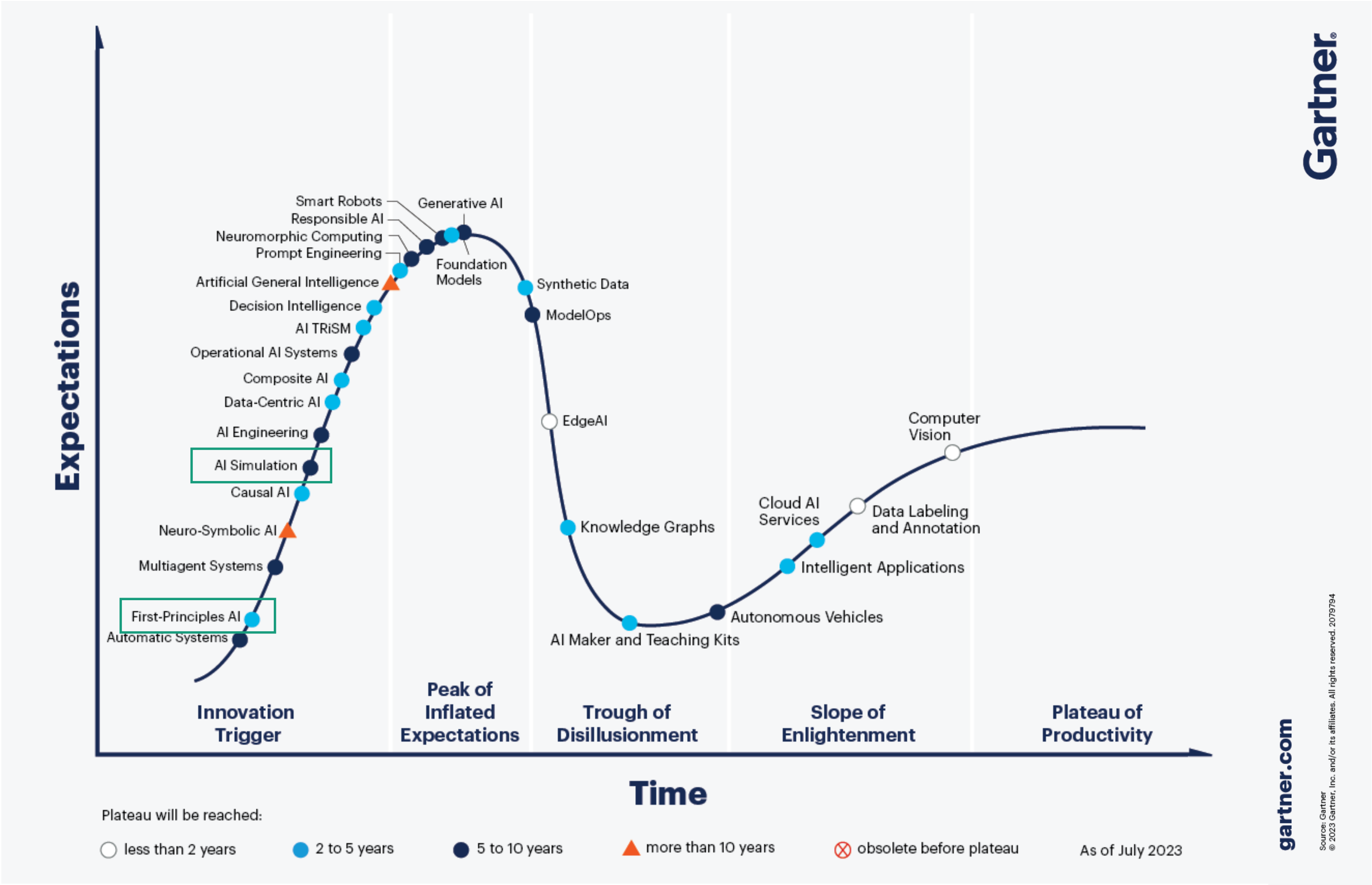

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⇒ **RL4Engineering**

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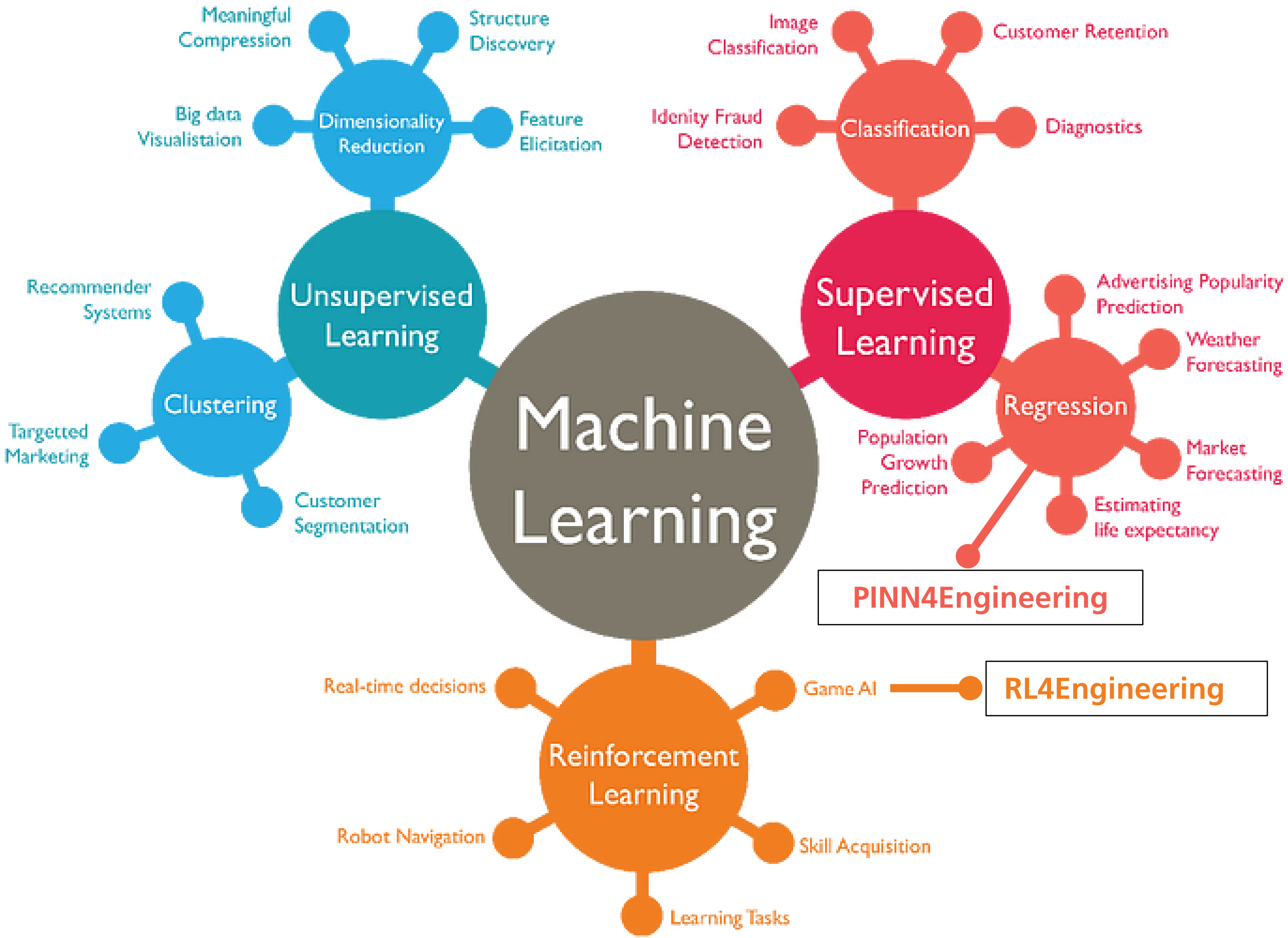

[1] https://medium.com/@wahlschwabe/künstliche-intelligenz-supervised-unsupervised-und-reinforcement-learning-eine-übersicht-4877b020c95b

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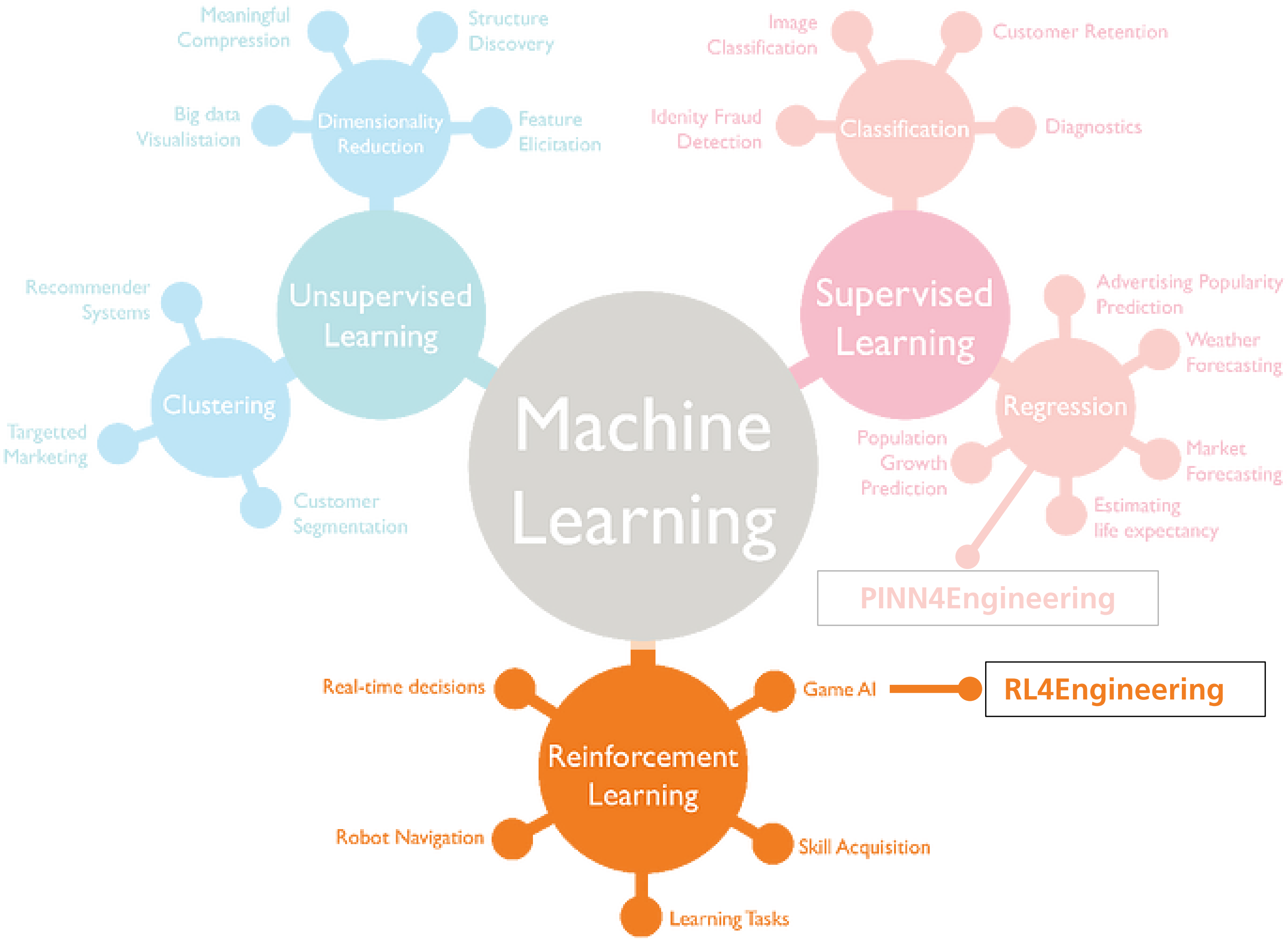

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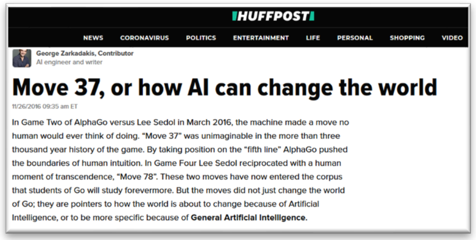
Reinforcement Learning

From "Game AI" to "RL4Engineering"

2016 - AlphaGo

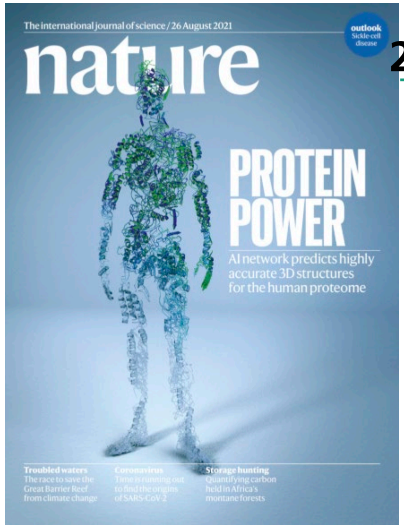

HUFFPOST

George Zarkadakis, Contributor
AI engineer and writer

Move 37, or how AI can change the world

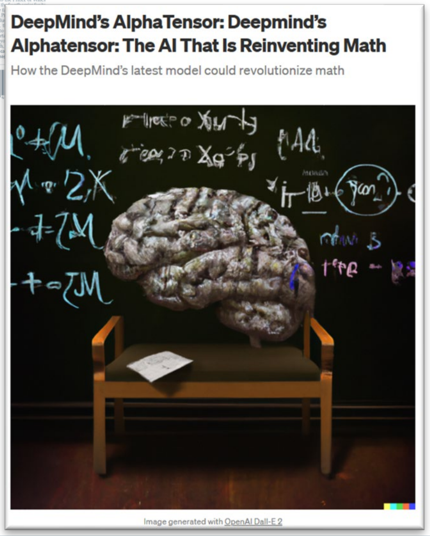
11/26/2016 09:35 am ET

In Game Two of AlphaGo versus Lee Sedol in March 2016, the machine made a move no human would ever think of doing. "Move 37" was unimaginable in the more than three thousand year history of the game. By taking position on the "fifth line" AlphaGo pushed the boundaries of human intuition. In Game Four Lee Sedol reciprocated with a human moment of transcendence, "Move 78". These two moves have now entered the corpus that students of Go will study forevermore. But the moves did not just change the world of Go; they are pointers to how the world is about to change because of Artificial Intelligence, or to be more specific because of **General Artificial Intelligence.**



2021 - AlphaFold

2022 - AlphaTensor



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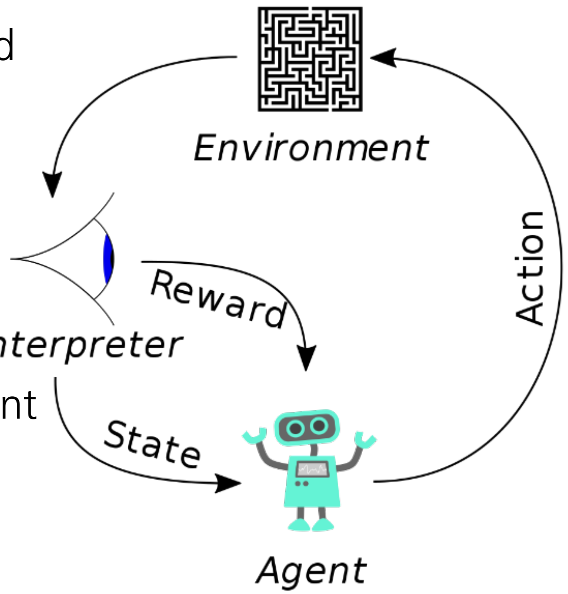
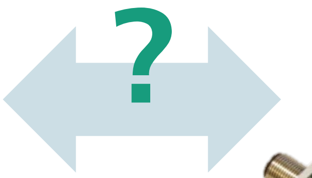
How to design engineering games?

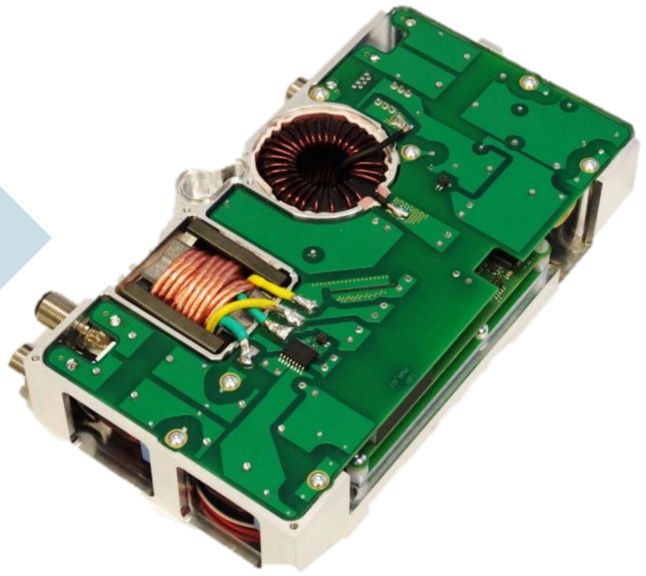
Assuming there is a sufficiently accurate data base and simulation model…

Challenge 1:
How to design engineering “games”?
- Design an “engineering” environment
- Define rules for actions in this environment
- Design an appropriate reward function for the agent

Challenge 2:
What is a proper reinforcement learning algorithm?
- Value-based, Policy-based, Model-based reinforcement learning?
- Exploration vs. Exploitation
- Continuous Learning vs. Catastrophic Forgetting







How to combine the general workflow for Reinforcement Learning with real world engineering problems?

https://en.wikipedia.org/wiki/Reinforcement_learning

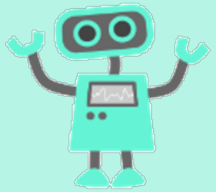
RL4Engineering

Gamification of electronic circuit design – General Strategy

L_r [uH]	L_m [uH]	C_r [nF]	k	f_1 [kHz]	f_2 [kHz]
0.1-100	0.1-100	10-10000	0.9-0.99	10-50	50-100

Actions define parameter values for next simulation

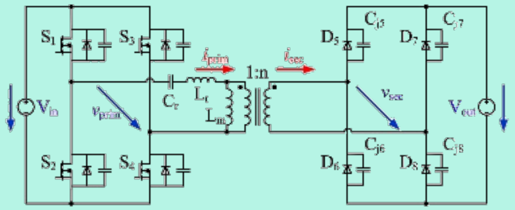
Action



RL-Agent

Proximal Policy Optimization (PPO) [Schulman 2017]

Environment



Simulation (FHA) of circuit (LLC) computes e.g. output power

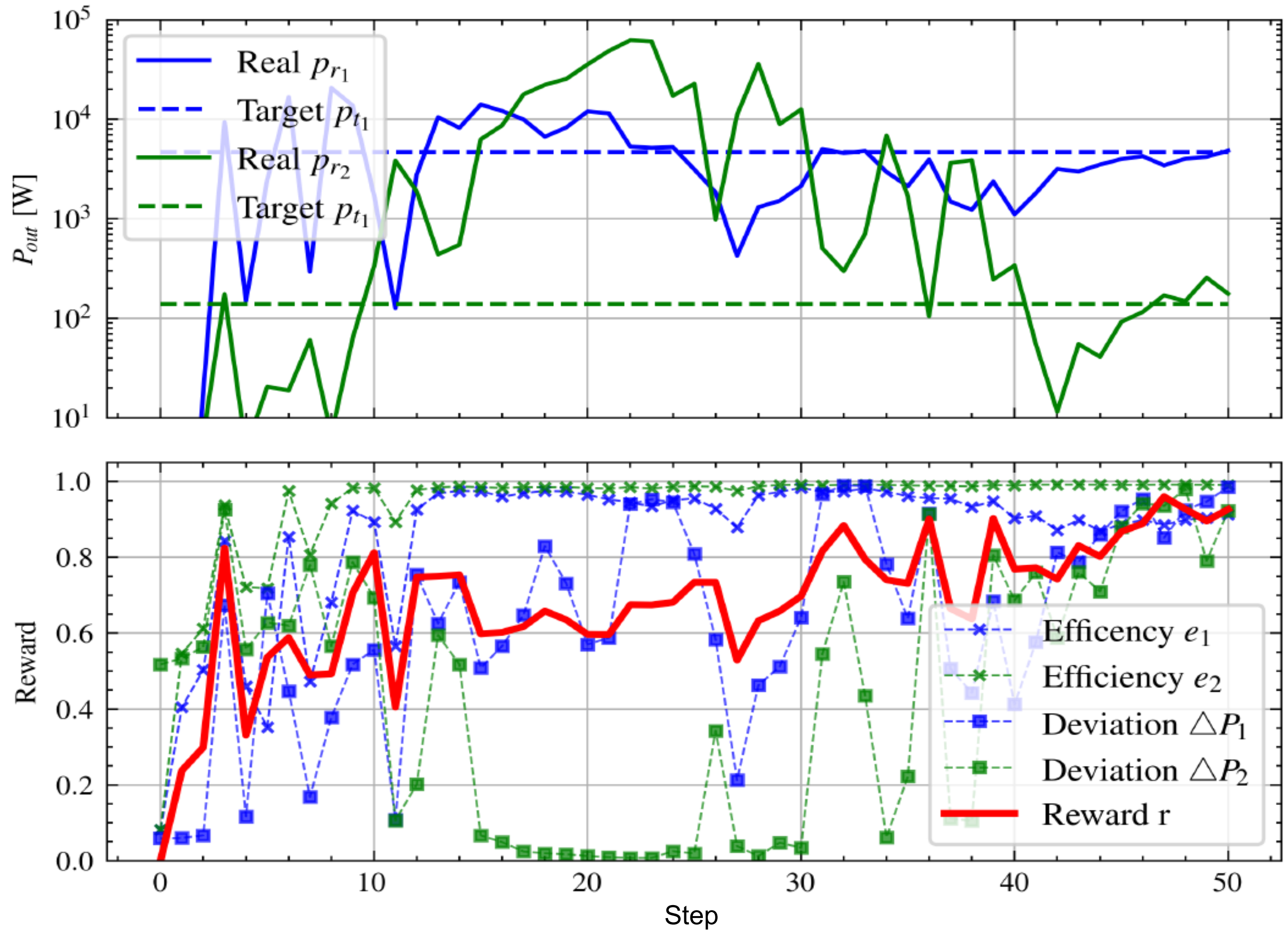
Next state, Reward

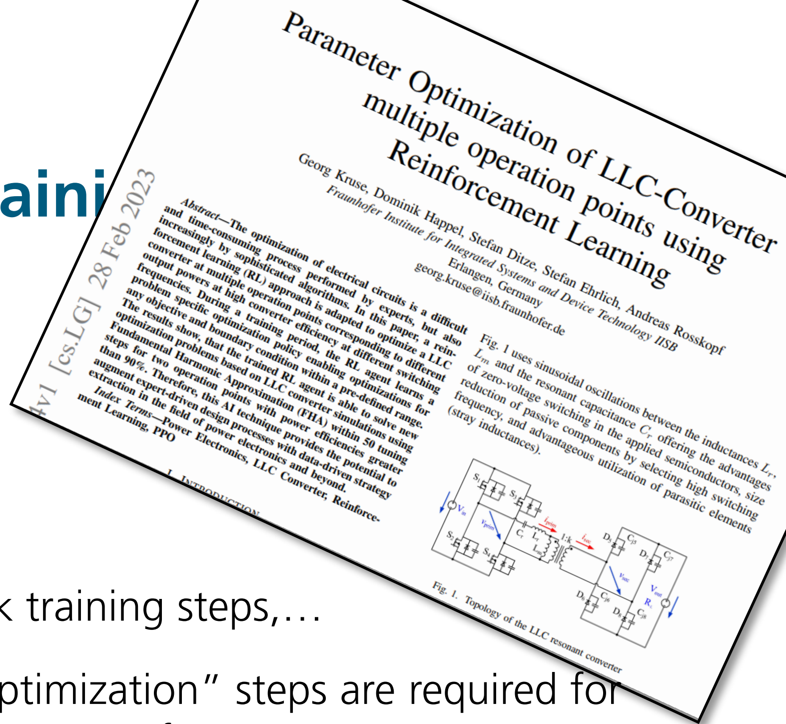
Reward:
Meet two output power values with high efficency.

$$r = \frac{1}{4}\left[e_1 + \underbrace{\left(1 - \frac{|p_{r_1} - p_{t_1}|}{p_{r_1} + p_{t_1}}\right)}_{\Delta P_1} + e_2 + \underbrace{\left(1 - \frac{|p_{r_2} - p_{t_2}|}{p_{r_2} + p_{t_2}}\right)}_{\Delta P_2}\right]$$

All in all 30.000 training steps with 50 circuit evaluations each

Gamification of electronic circuit design – Result after traini





Result after 30k training steps,…

- only 50 “optimization” steps are required for matching two specific target power outputs within a wide range of output power ranges.
- Targeted output power values have been met.
- Efficiency for both OP greater 90%.

Details at arxiv.org/pdf/2303.00004.pdf

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Fight for diversity

- Reinforcement learning is a rising star for engineering problems, but currently lacks diversity in solution candidates.
- In very sparse solution spaces, the first successful RL-trajectory shape the solution strategy.

⇒ New, fast exploration strategies are needed

⇒ Continuous Adaptive Random sampling (CARS)

RL4Engineering

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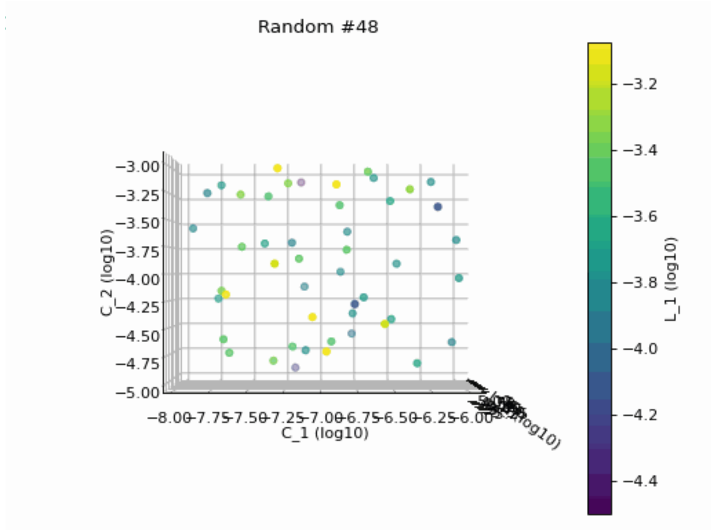
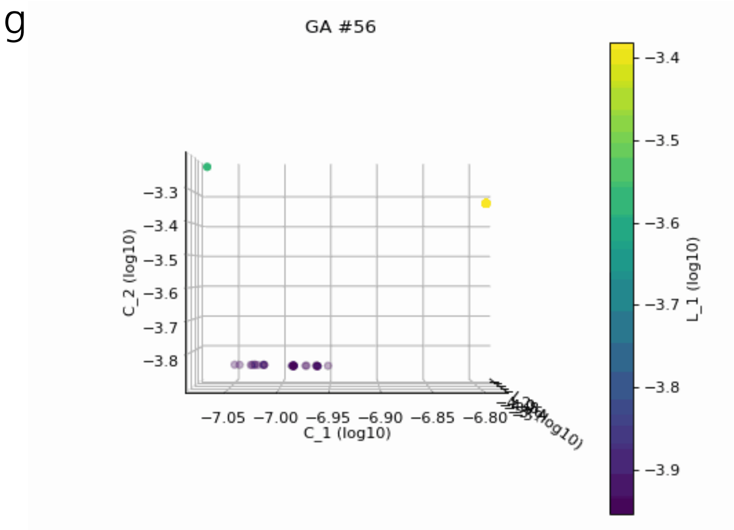
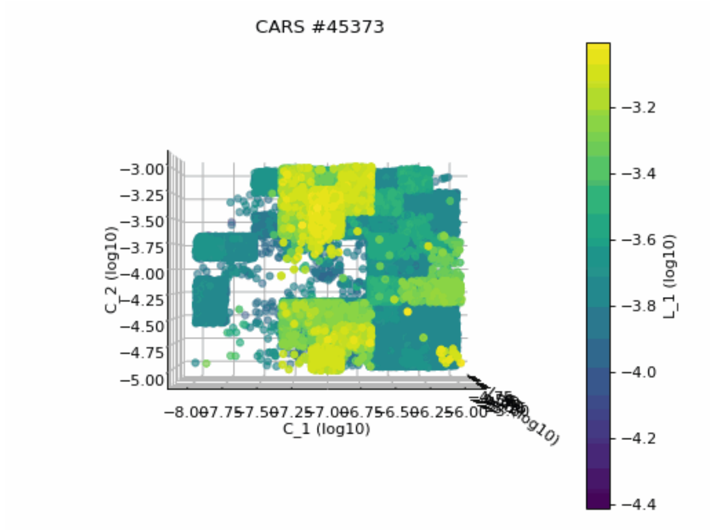
Challenge:
Find valid samples of an LLC-Converter in 1 hour

	Total Samples	Valid Samples
Random	12,000,000	48
GA	19,139	56
CARS	2,702,703	45,373





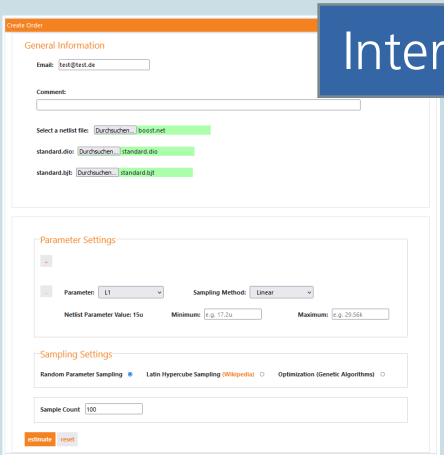


RL4Engineering

Gamification of electronic circuit design – on the way to online-service (SaaS)

SchoKI
www.schoki.app

Interface

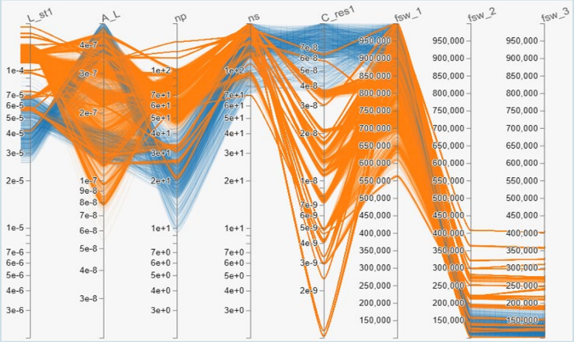


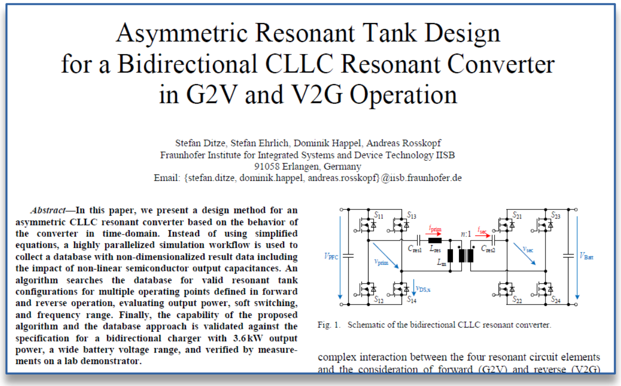
Design

Sampling
- Random
- GAs
- CARS
- Reinforcement Learning

Simulation
- LTspice
- FHA

Results





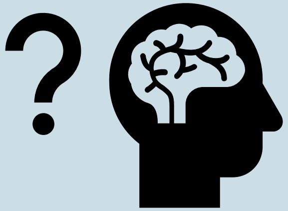
Asymmetric Resonant Tank Design
for a Bidirectional CLLC Resonant Converter
in G2V and V2G Operation

Stefan Ditze, Stefan Ehrlich, Dominik Happel, Andreas Rosskopf
Fraunhofer Institute for Integrated Systems and Device Technology IISB
91058 Erlangen, Germany
Email: {stefan.ditze, dominik.happel, andreas.rosskopf}@iisb.fraunhofer.de

***Abstract*—In this paper, we present a design method for an asymmetric CLLC resonant converter based on the behavior of the converter in time-domain. Instead of using simplified equations, a highly parallelized simulation workflow is used to collect a database with non-dimensionalized result data including the impact of non-linear semiconductor output capacitances. An algorithm searches the database for valid resonant tank configurations for multiple operating points defined in forward and reverse operation, evaluating output power, soft switching, and frequency range. Finally, the capability of the proposed algorithm and the database approach is validated against the specification for a bidirectional charger with 3.6 kW output power, a wide battery voltage range, and verified by measurements on a lab demonstrator.**

Fig. 1. Schematic of the bidirectional CLLC resonant converter.

complex interaction between the four resonant circuit elements and the consideration of forward (G2V) and reverse (V2G)



Engineer

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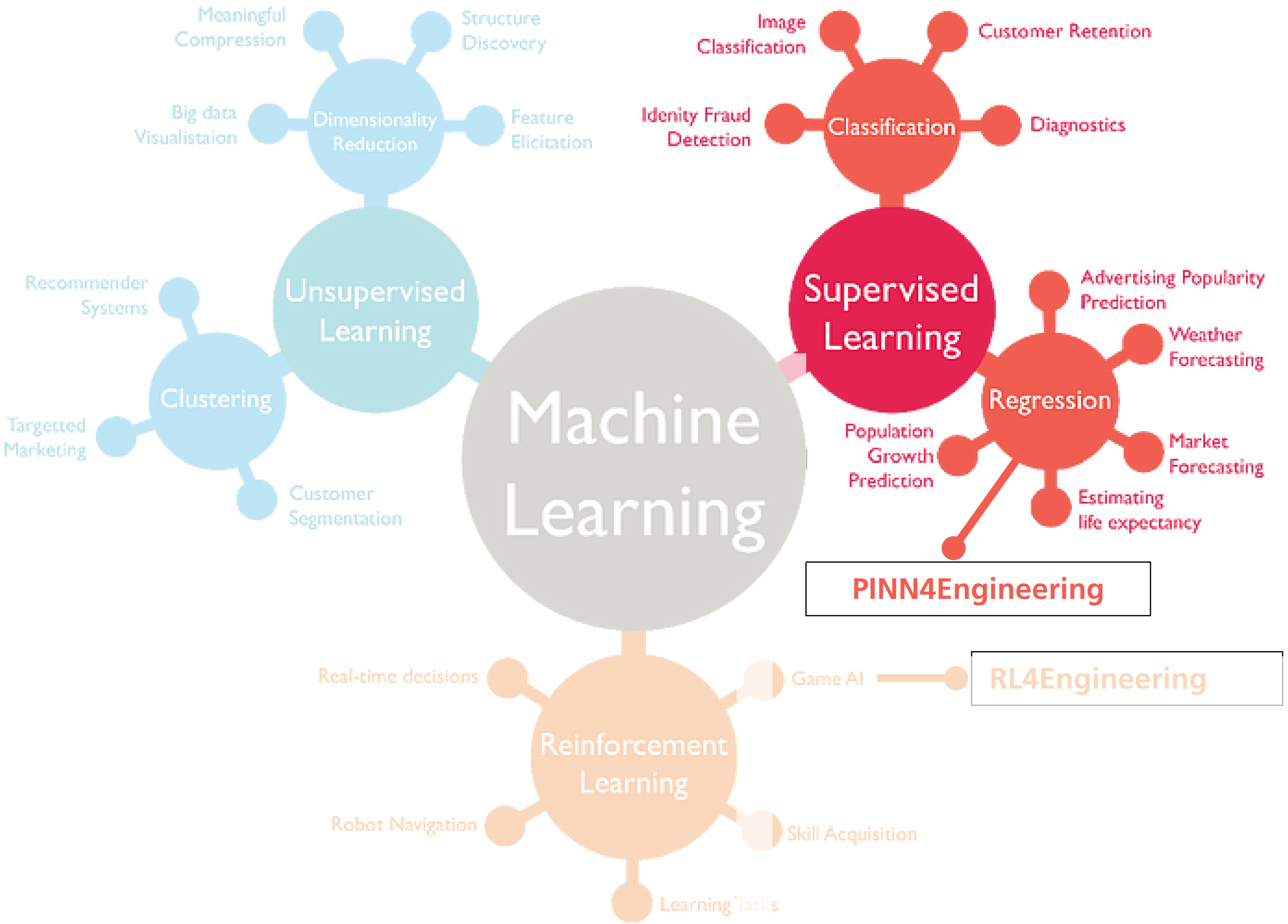

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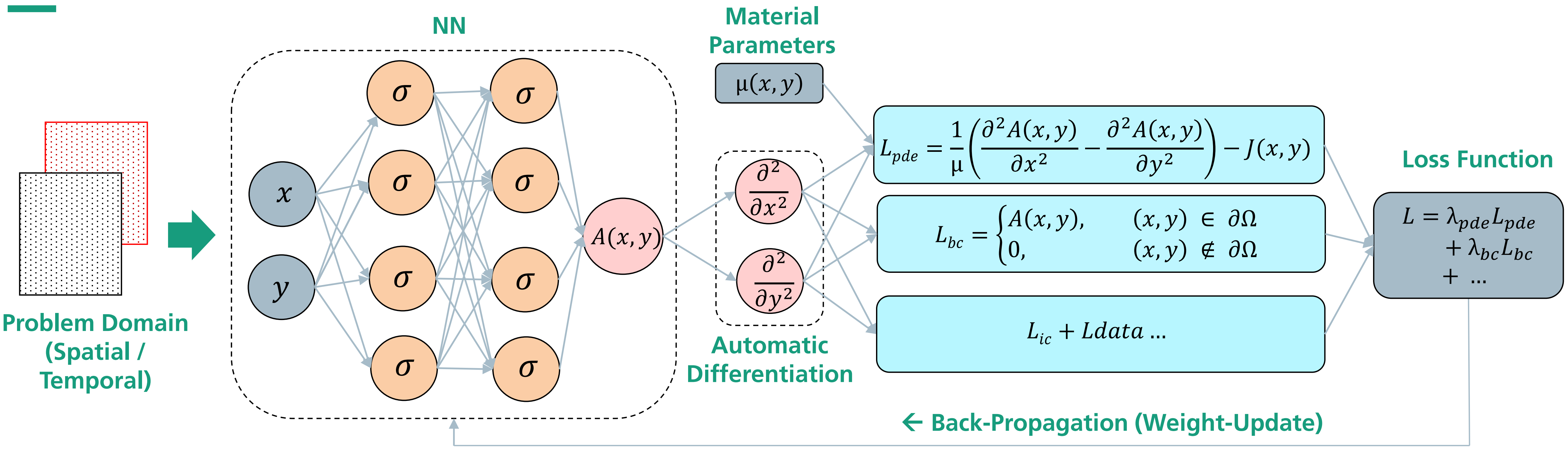
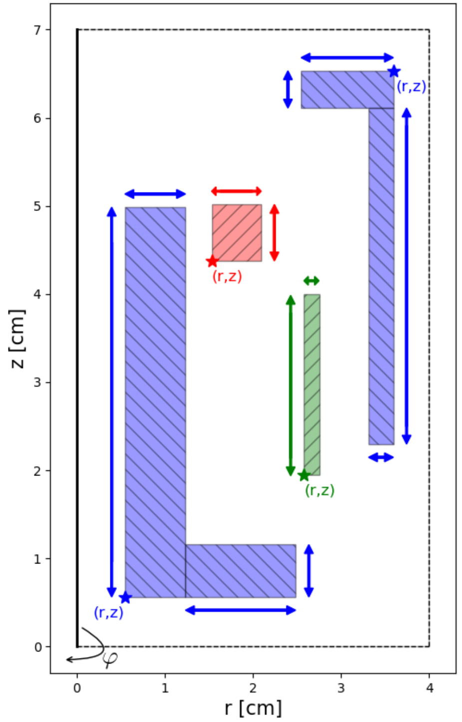
How to implement physical laws in NN?

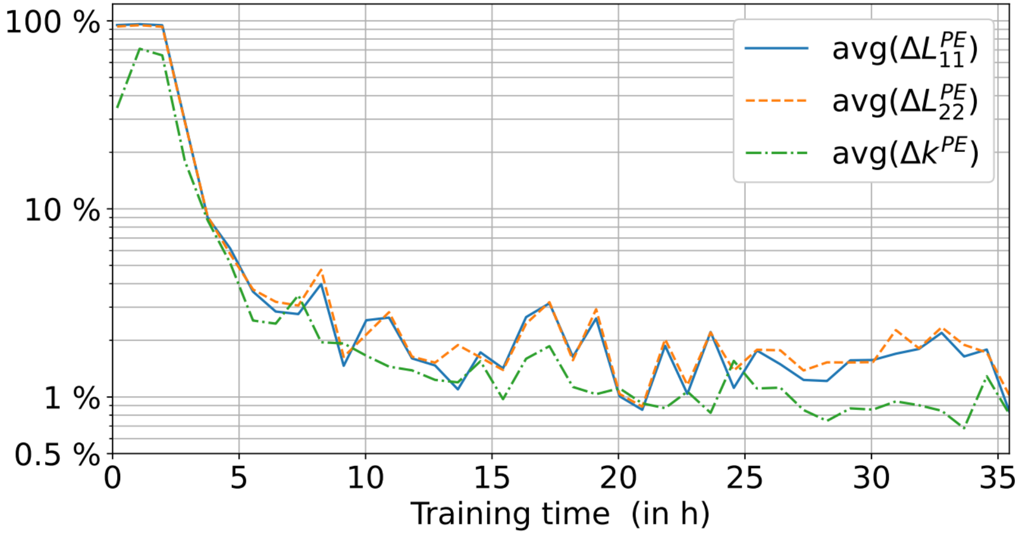


PDE (Quasistatic Maxwell Eq.)	$\frac{1}{\mu}\left(\frac{\partial^2 A(x,y)}{\partial x^2} - \frac{\partial^2 A(x,y)}{\partial y^2}\right) = J(x,y)$
Boundary Condition	$A(x,y) = 0 \qquad (x,y) \in \partial\Omega$
Initial/Interface-Conditions, Data etc.	…

- PINN as Approximator for PDE-solution
- Physical Constraints incorporated in Loss-Function
- Shallow Networks of e.g. 3x300 Nodes sufficient

PINN for EMAG: Inductance extractor





	$avg(\Delta L_{11}^{PE})$	$avg(\Delta L_{22}^{PE})$	$avg(\Delta k^{PE})$
ConvPINN	0.84%	1.02%	0.81%

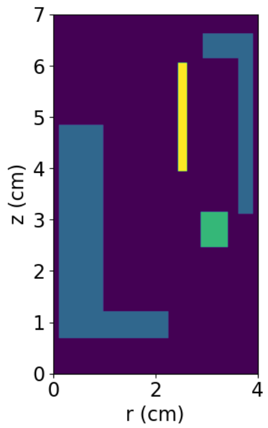
Engineering challenge
Optimal coil design for an inductive power transfer system.

Geometric parameter space
18 degrees of freedom, two simulations with different coil excitation.

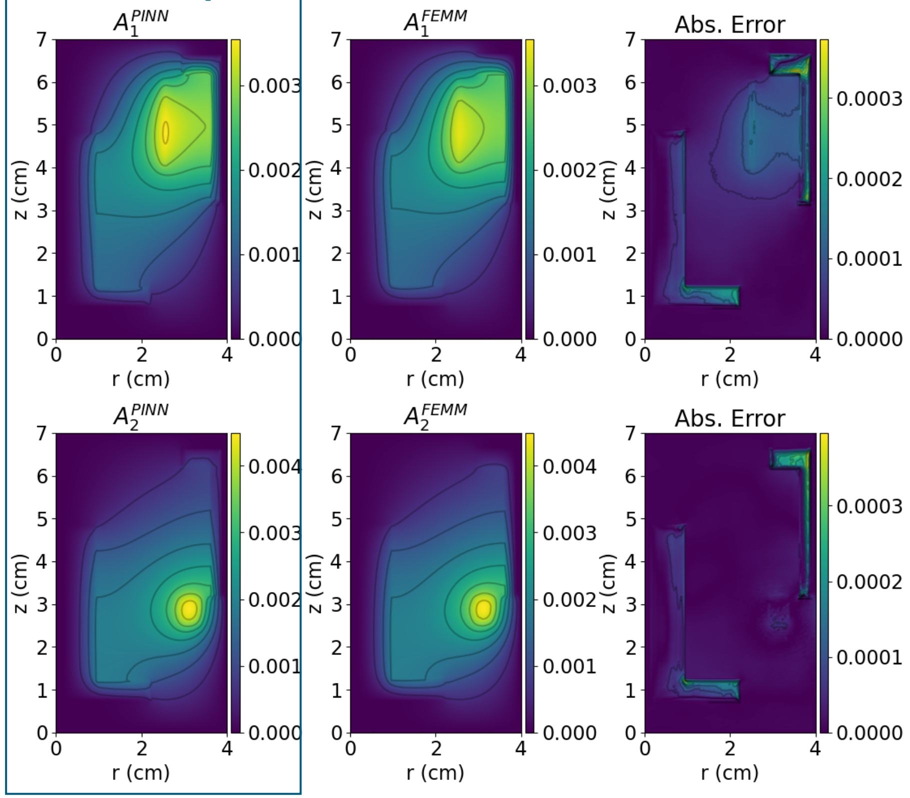
Convergence profile of the PINN
After one training day on one GPU inductance and coupling is approximated with less than 1-2% deviation from reference.

PINN for EMAG: New dimension of speed

Geometry Input

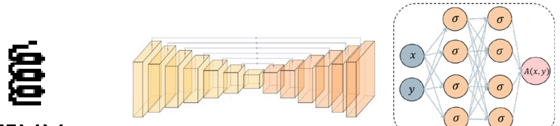


Field Output



Internal results

The spatial magnetic vector potential is approximated and integrated.



	Reference Similation	ConvPINN	FC – PINN
Setup	382 ms (geom., phy.)	0.4 ms (2D array)	0.06 ms (r,z, λ)
Solve / Predict	534 ms	8.1 ms	0.4 ms
Total Inference	916 ms	8.5 ms	0.5 ms

x 100

x 2.000

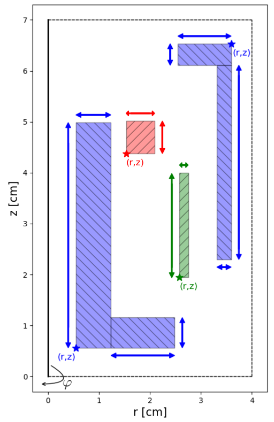
Optimizations with more than 200k evaluations are already faster via PINN compared to FEM.

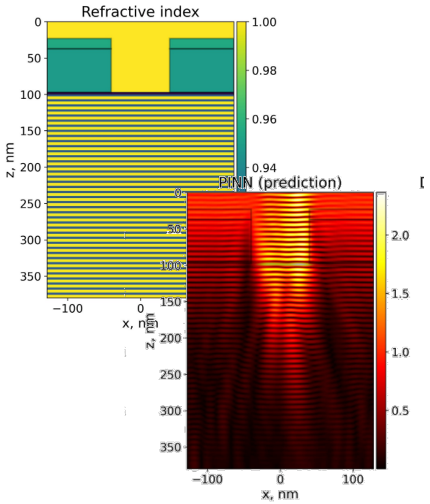
Results & Opportunities

New ratio of problem complexity and solution speed.

PINN4Engineering

Current IISB fields of applications





EMag Inductance Extraction

- Physics: Quasistatic Maxwell Eq., 2D
- Application:
  - Optimization of Inductive Systems
- Benefit:
  - Speed -> Optimization

Platinum Diffusion in Silicon

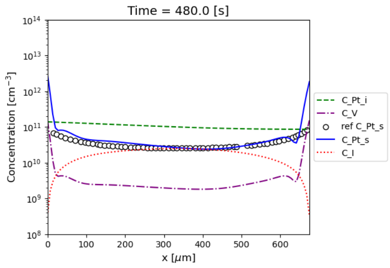
- Physics: Reaction-Diffusion system,1D
- Application:
  - Optimization of Semiconductor Devices, Param. Reconstruction
- Benefit:
  - Complex Physics + Data

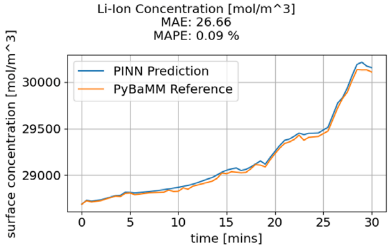
Mask Simulation

- Physics: Helmholtz wave eq., 3D
- Application:
  - Generalized PINN to simulate light scattering in 3D
- Benefit:
  - Speed + Complex Physics

Battery SOC-Approximation

- Physics: Diffusion of Li-Ion, 1D
- Application:
  - SOC / SOH prediction
- Benefit:
  - Speed -> Micro-Controller
  - Data Enhancement





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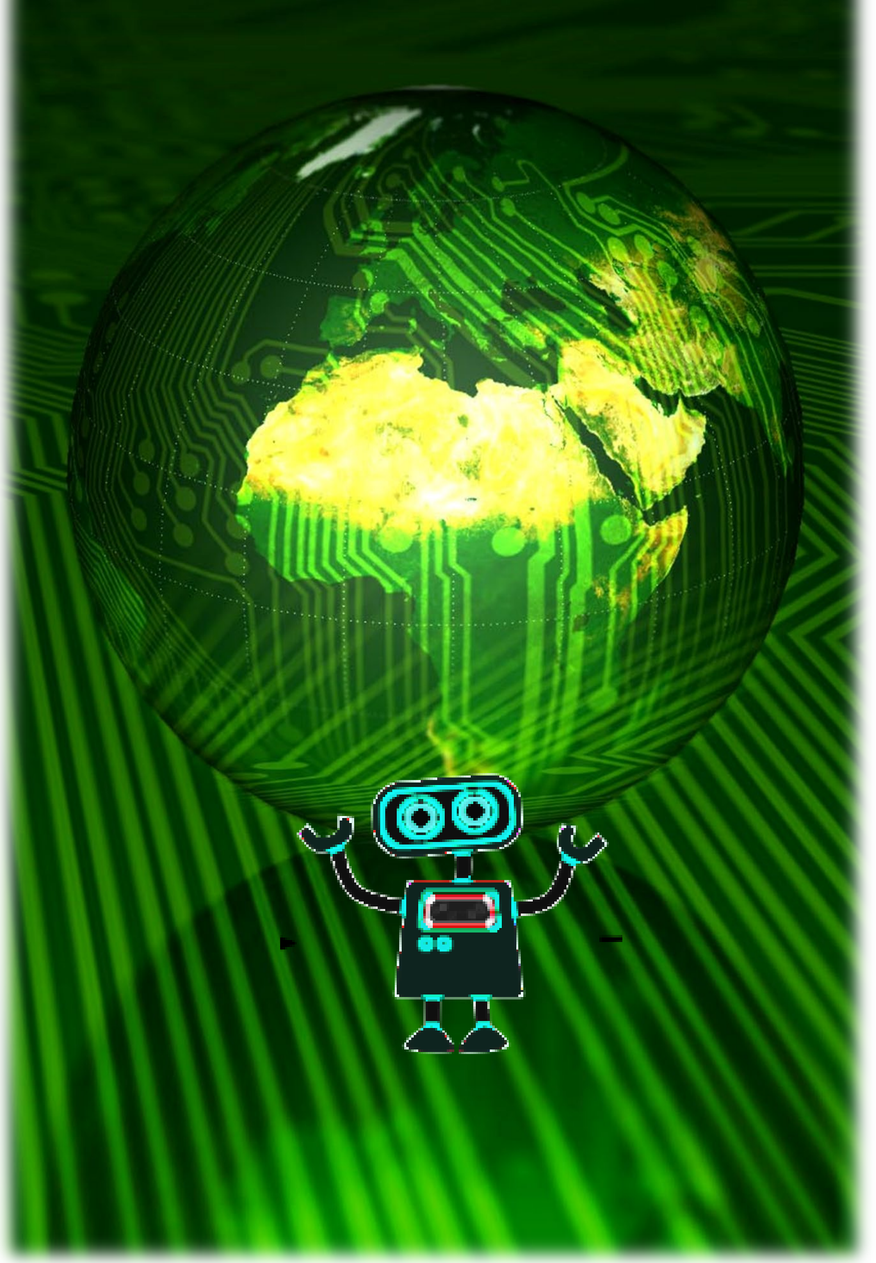
Conclusions

- Engineering problems are increasingly in the focus of AI and ML approaches
- Initial success stories of Reinforcement Learning in the domain of gaming have been adapted to mathematical and engineering problems. Advances in engineering game design, generalizability, and diversity offer the potential to catch up with domain experts in the next decade.
- PINNs are on the move to highly accurate, ultra-fast domain-specific simulators. In the next few years, this methodology will enormously improve the quality and application of simulations and metamodels.
- “Physics and/or data science?”
  Physics, data science and measured data will close the gap between simulation and experiment and will provide more accurate simulators and new business models for digital solutions.



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Contact

Dr. Andreas Rosskopf
Head of AI-augmented Simulation
Tel. +49 9131 761 153
andreas.rosskopf@iisb.fraunhofer.de