Future Research Pharma

Practical insights into the use of AI in industry

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Tensor AI Solutions GmbH

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TENSOR SOLUTIONS

We create explainable AI …

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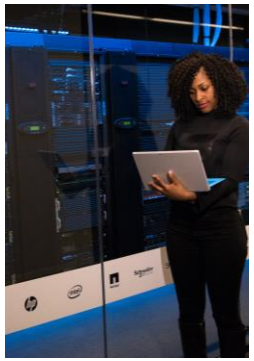
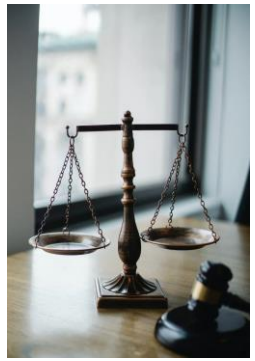
EXPLAINABLE INTELLIGENCE

… to control

… to discover



… to improve



… to justify

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2021

Bundesministerium für Wirtschaft und Klimaschutz

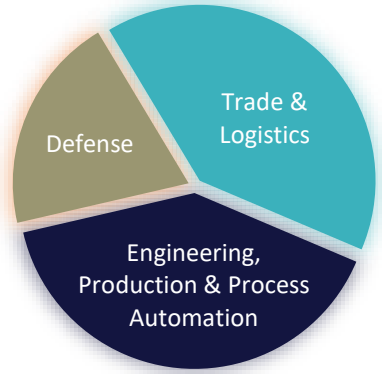
eXIST Existenzgründungen aus der Wissenschaft

universität ulm

ESF Europäischer Sozialfonds für Deutschland

Europäische Union

Zusammen. Zukunft. Gestalten.



2025

BRADY

LIEBHERR

Einstein Automotive e.V.

Bosch Engineering

BOSCH Invented for life

HENSOLDT Detect and Protect.

optimed

Elbit Systems Deutschland

HBC. Hochschule Biberach University of Applied Sciences

State of AI

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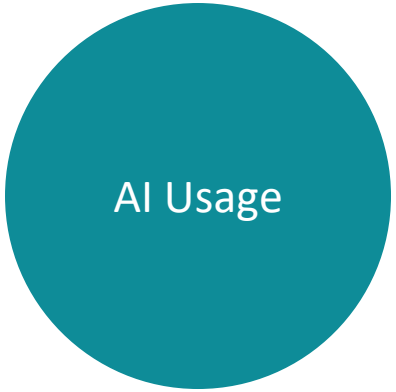
34 Mio.
Number of AI generated images (daily, worldwide)

78% of companies surveyed use AI in at least one business function



5% of the US power is consumed by data centers

70%
Estimated annual increase of GenAI power demand

Healthcare AI market
has doubled since 2023

https://www.morganstanley.com/ideas/ai-energy-demand-infrastructure (last visited 2025-04-30)
https://www.mckinsey.com/capabilities/quantumblack/our-insights/the-state-of-ai (last visited 2025-04-30)
https://www.forbes.com/sites/bernardmarr/2025/03/10/15-mind-blowing-ai-statistics-everyone-must-know-about-now/ (last visited 2025-04-30)

EU: Between GPT and Regulations

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AI Boom

- Launch of ChatGPT opened the door for a multitude of **AI applications**
- **High expectations** of end users and industry
- Unprecedented **opportunities** and **challenges**

Regulations

- Commitment to a **responsible** and **reliable** use of technology
- **Risk-oriented** perspective
- **Rapid development** complicates legislations

Théâtre D'opéra Spatial: Image by Jason M. Allen - Colorado State Fair, Public Domain, https://commons.wikimedia.org/w/index.php?curid=122602647 (last visited 2025-04-30)

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Perspective in Pharma

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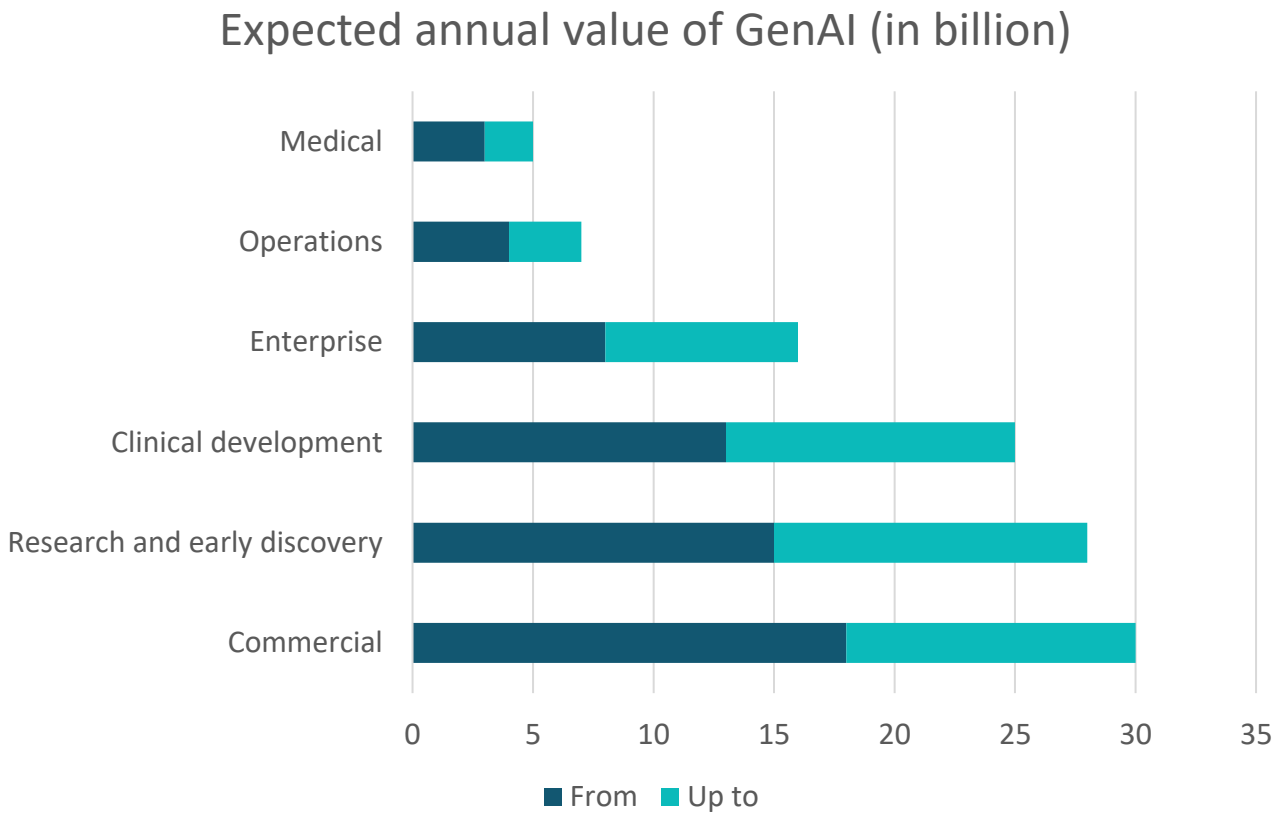

*"Gen AI models account for only about **15 percent** of a typical project effort […].*

*Most of the work involves adapting models to a **company's internal knowledge base** and **use cases.***

*That is particularly true in the pharmaceutical industry, given the **complexity of its data** and the uniqueness of its **regulations** and **technology**."*

https://www.mckinsey.com/industries/life-sciences/our-insights/generative-ai-in-the-pharmaceutical-industry-moving-from-hype-to-reality#/ (last visited 2025-04-30)

EU: Application Areas

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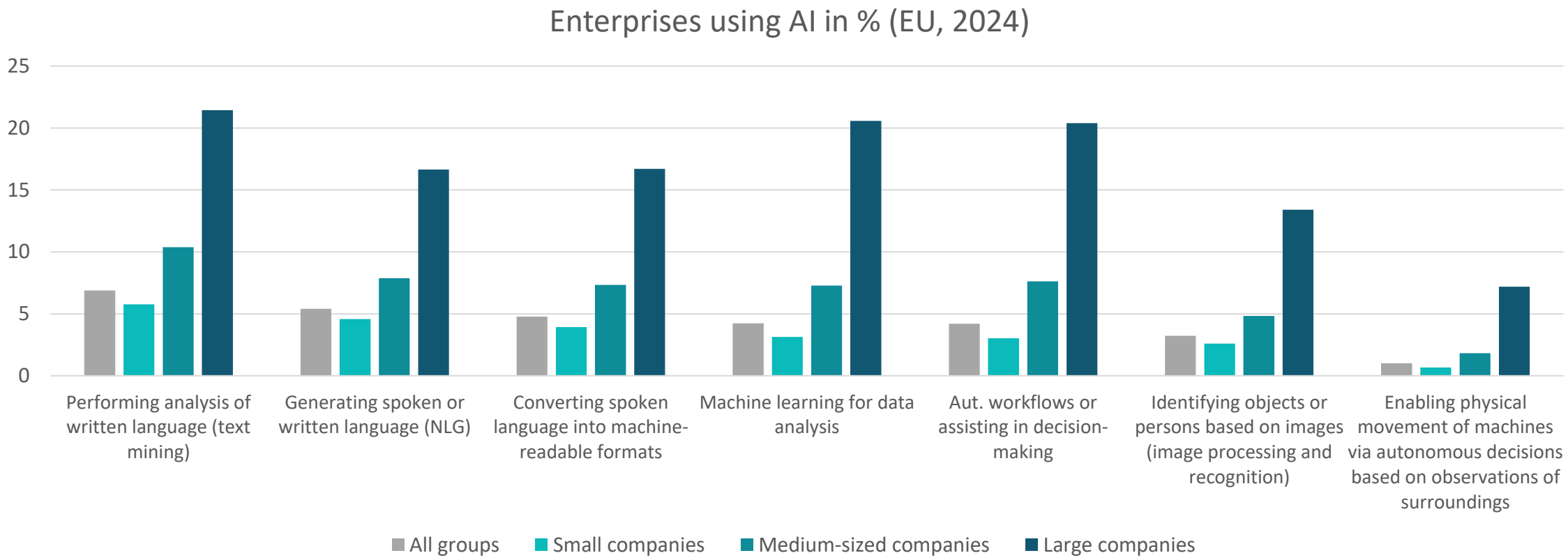

https://ec.europa.eu/eurostat/statistics-explained/index.php?title=Use_of_artificial_intelligence_in_enterprises (last visited 2025-04-30)

Use Case: Quality Control

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- Quality depends on different **process** and **material parameters**
- Classical QC: **reactive**, **time-delayed** and often **manual**
- Established approach: **Automated visual inspection** (image processing)
  - **Reasons** for quality deviations frequently **unknown**
  - Especially **complex patterns** often remain undetected

➢ **ML** offers unique insights if **models can be explained**

➢ Similar requirements in **multiple use cases**, e.g.

- ➢ Steel production
- ➢ Chemical coating
- ➢ Real-time release testing

Example: Real-time Release Testing

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> *"The ability to **evaluate** and **ensure** the **quality of in-process and/or final product** based on **process data**, which typically include a valid combination **of measured material attributes** and **process controls**."*
>
> - ICH, 2009. Q8(R2) Pharmaceutical Development (step 5)

- Approach: data-based **surrogate models** to measure dissolution
- Typical methods are **multi-linear regression** (MLR) and **partial least square** (PLS) regression

➢ Complex models like **neural networks** were studied but frequently **lack transparency** (black box)

➢ Often **manual selection** and **comparison** of input data

Galata, Dorián László, et al. "Real-time release testing of dissolution based on surrogate models developed by machine learning algorithms using NIR spectra, compression force and particle size distribution as input data." *International journal of pharmaceutics* 597 (2021): 120338.

Explainable AI

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*"**Machine learning** systems automatically learn **programs from data**"*

Domingos, Pedro. "A few useful things to know about machine learning." *Communications of the ACM* 55.10 (2012): 78-87.

- Usual trade-off: model **complexity** vs. **transparency**
- Explainable AI (XAI) aims at making the **learned patterns visible/understandable**

- Explanation **scopes**:
  - **Local explainability** (individual predictions)
  - **Global explainability** (full model)
- Examples: **Local explainability**
  - Sensitivity maps
  - SHAP values (individual feature contribution)

Prediction: Canyon

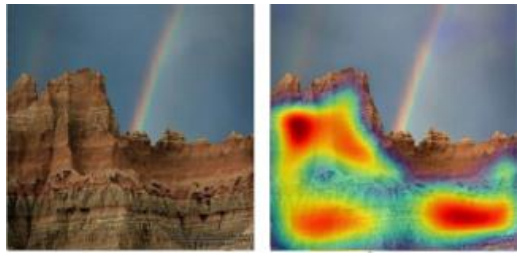
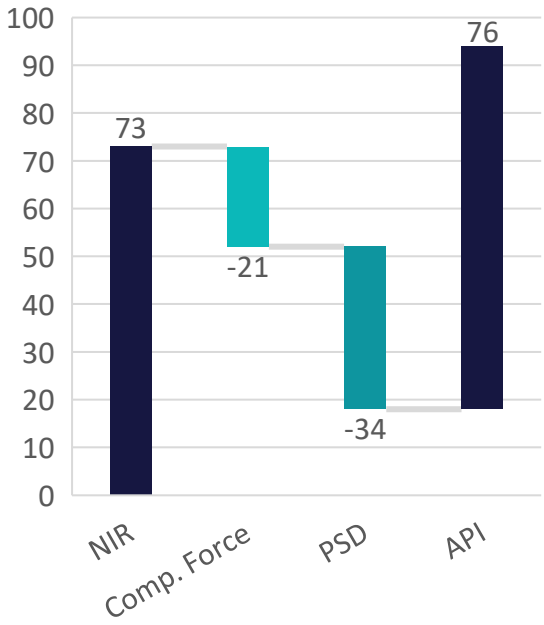


Image source: [1]

Quality prediction: **92%**



Exemplary data and visualization

1. Selvaraju, Ramprasaath R., et al. "Grad-CAM: Visual Explanations from Deep Networks via Gradient-based Localization." *arXiv preprint arXiv:1610.02391* (2016).
2. Topalian, Romain, et al. "Safe-by-Design Strategies for Intranasal Drug Delivery Systems: Machine and Deep Learning Solutions to Differentiate Epithelial Tissues via Attenuated Total Reflection Fourier Transform Infrared Spectroscopy." *ACS Pharmacology & Translational Science* 8.3 (2025): 762-773.

Tensor Network Technology

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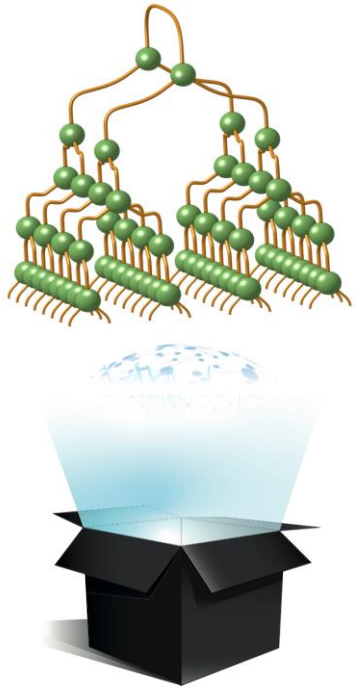
***Quantum** by nature*
***Transparent** by design*

Control information

- Traceability of learned patterns
- Measurability of relevant data for AI decisions
- Integration of expert knowledge or regulatory constraints

Origin

- Used to simulate many-body quantum systems
- Information theory-based reduction of dimensionality



Improve efficiency

- Reduction of data to the most relevant for decision-making
- Compression of AI models after training for an optimal balance between accuracy and speed

Use Cases

- Object detection in real-time
- Robust processing of satellite data
- Particle recognition from high-energy physics data

Felser, Timo, et al. "Quantum-inspired machine learning on high-energy physics data." *npj Quantum Information* 7.1 (2021): 111.

How transparent is enough?

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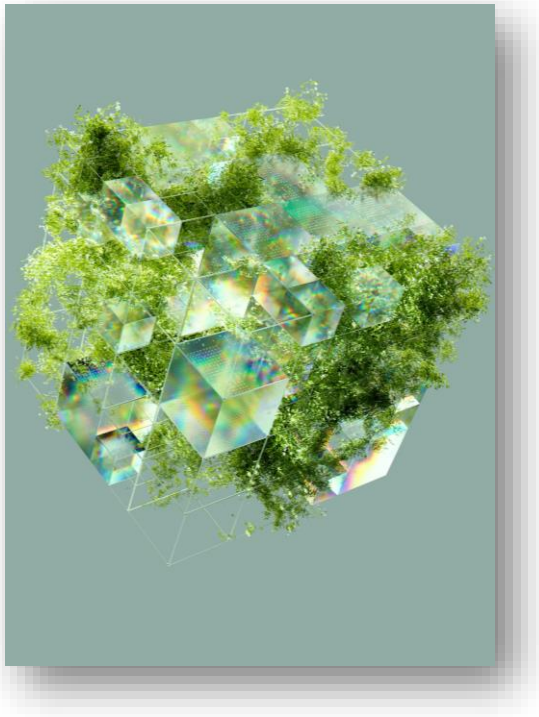
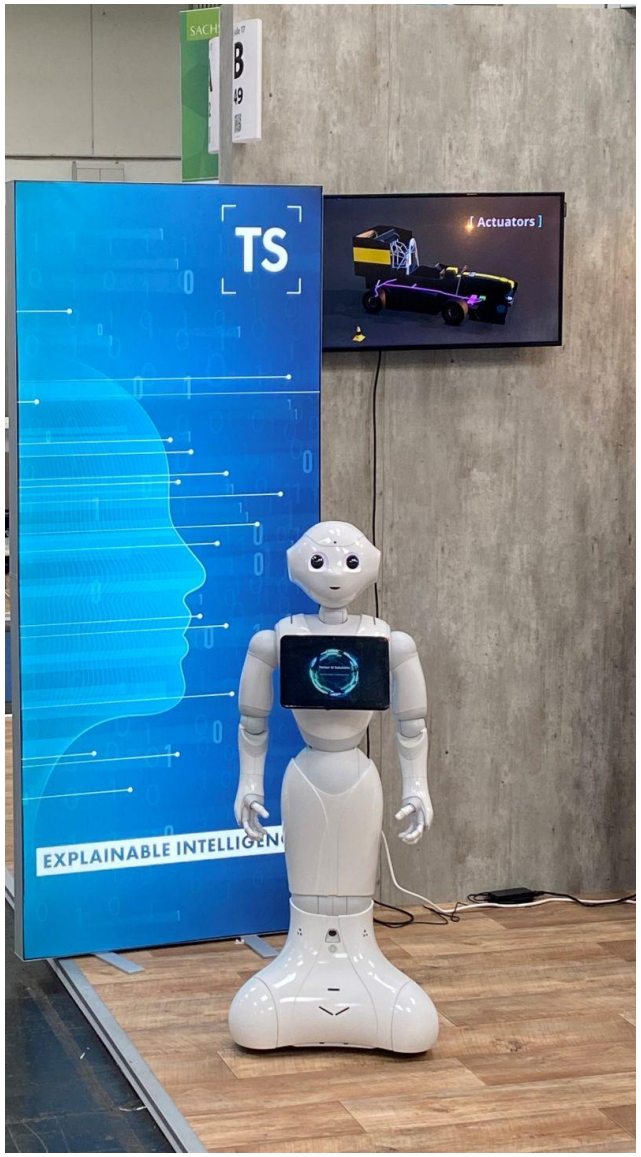


- **Limited data** and **high** (regulatory) **standards**
  - E.g. GxP (GAMP, GMP, GCP, etc.)
- Clarify similar XAI **obligations** for different **use cases**
  - What information needs to be accessible?
  - How is explainability assessed?
  - Which decisions require a human in the loop?

➢ **Standardize** explainability to enable **reliable** and **assessable models**

➢ **Synchronize regulations** and **XAI standards** across industries

DIN ZERTIFIZIERTE KI
Qualität sichern. Fortschritt gestalten.



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Thank you for your attention!

EXPLAINABLE INTELLIGENCE

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