Institute for Machine Learning

Bachelor Info Event
Dr. Daniel Klotz and Dr. Johannes Kofler
24 January 2022

JOHANNES KEPLER
UNIVERSITÄT LINZ

Institute for Machine Learning & LIT AI Lab

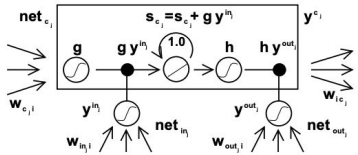
JOHANNES KEPLER UNIVERSITÄT LINZ

- Head: Prof. Sepp Hochreiter
- 2 Assistant Professor & 8 Postdocs
- More than 35 PhD Students
- Research focus: Machine Learning, Deep Learning
- Initiated Austria’s first AI Study Program at JKU
- LIT AI Lab at JKU:
  - 6 groups (Deep Learning, Computer Vision, Logical Reasoning, Pervasive Computing, Software Engineering, Symbolic Computing)
  - PhD School, ELLIS Unit

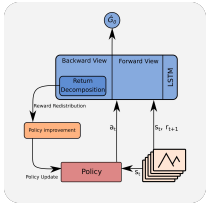
Bachelor Theses

- Find a topic that can be supervised by our Institute
- Topic areas: see our website and next slides
- Contact institute (secretary@ml.jku.at) and/or Dr. Sebastian Lehner (s.lehner@ml.jku.at)
- Ideally (but not necessarily) an extension of the “Practical Work in AI” (5th semester) project
- Research:
  - Familiarize with the relevant literature
  - Formulate project objectives, research goals
  - Design and conduct computational experiments
  - Analyze experimental results and interpret them
- Thesis:
  - scientific style & structure
  - 15-30 pages
  - standardized layout
- No oral presentation

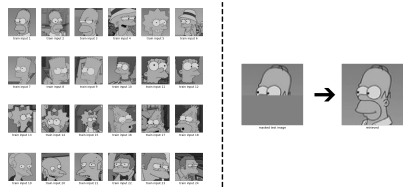
AI research groups at Institute for Machine Learning



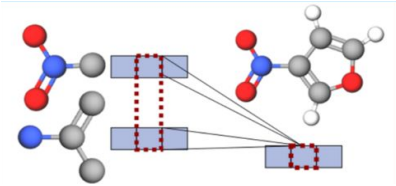
Deep Learning



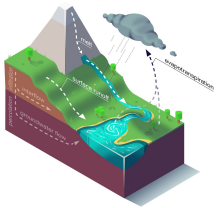
Reinforcement Learning



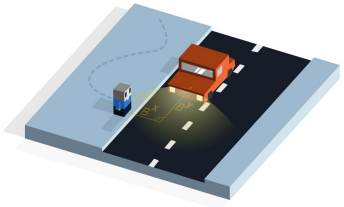
Hopfield networks



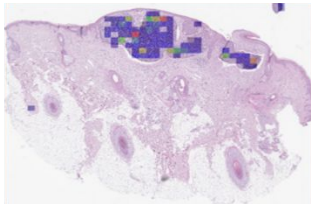
AI in Drug Discovery



AI 4 Earth



AI 4 Driving



AI in Healthcare

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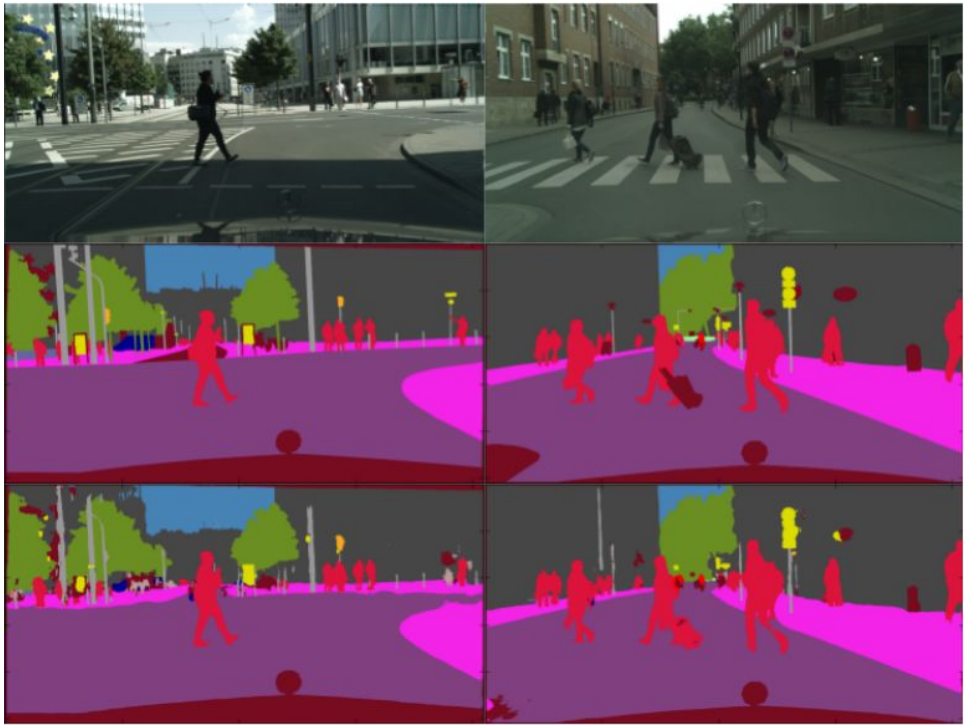
Incomplete list of projects

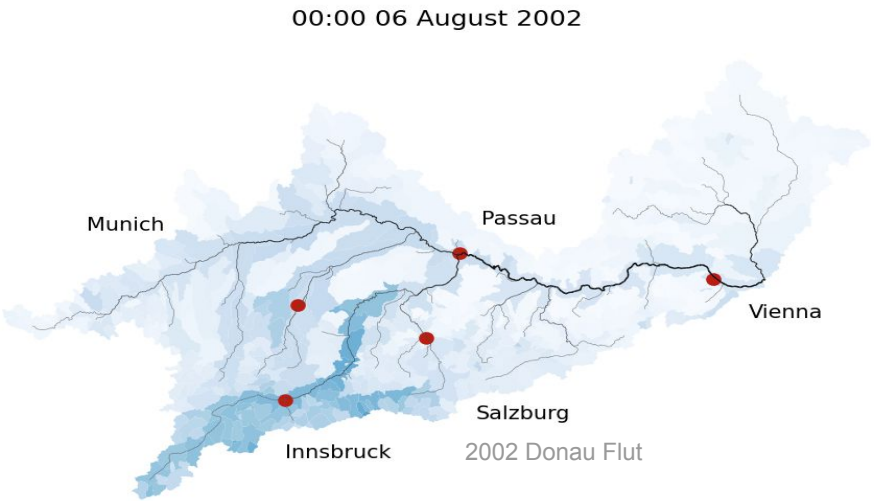
- Semantic segmentation for autonomous driving
- AI for climate and environment
- Machine learning for physics simulations
  - Particle flows simulations and particle-particle interactions
  - Molecular modeling
- AI in drug discovery and chemistry; machine learning for molecules
- SoC design, Logistics: resilient warehouse
- CLOOB: connecting text and images

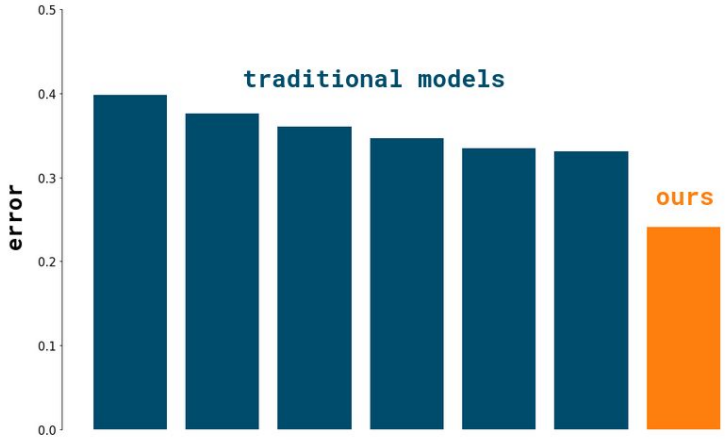
Semantic segmentation for autonomous driving

- AI methods to enable self-driving cars
- Camera images have to be segmented into different areas (roads, other cars, …)
- Fast and accurate methods developed



AI for climate and environment

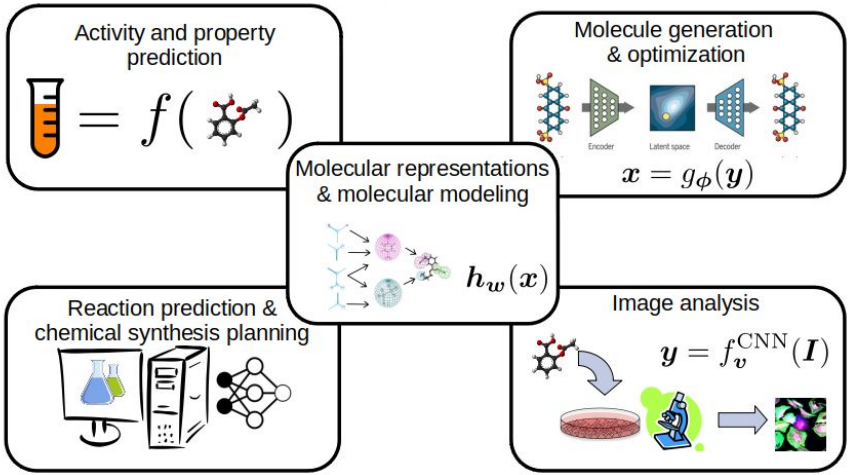




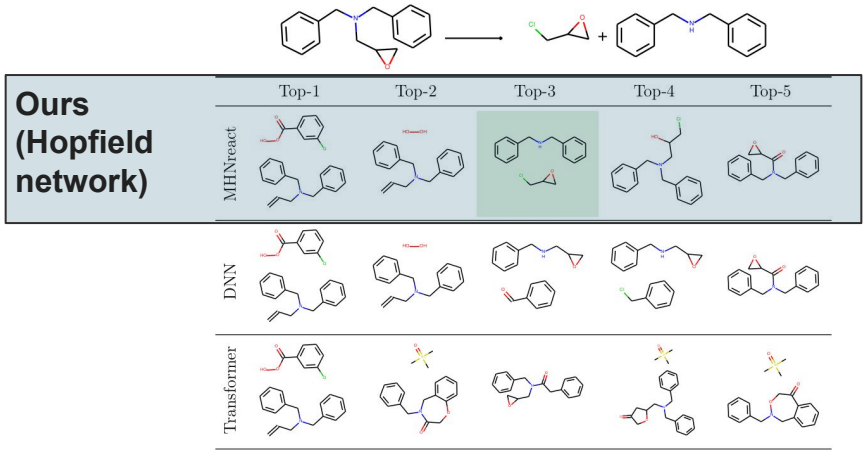
- Modelling environmental processes to guide decision making and better use of natural resources.
- Use of a wide range of environmental data (from weather data, land-surface characteristics, satellite observations) to make simulations and/or forecasts.

- Our models currently provide the best predictions over a variety of problem settings and metrics

AI in drug discovery and chemistry, ML4Molecules



- Finding new drugs with AI methods
- AI supports chemists at developing drugs
- Machine learning and Deep Learning has strongly improved computer-aided drug discovery

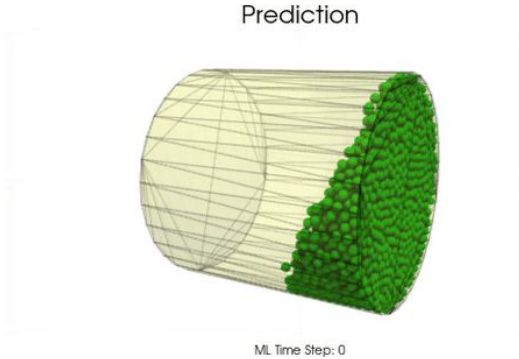


- Example: Hopfield networks predict products or reagents of chemical reactions

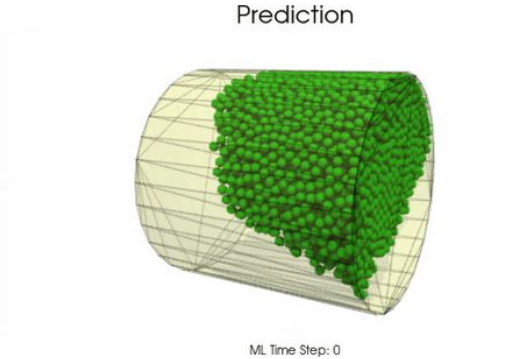
Seidl, P., Renz, P., Dyubankova, N., Neves, P., Verhoeven, J., Segler, M., ... & Klambauer, G. (2021). Modern Hopfield Networks for Few-and Zero-Shot Reaction Template Prediction. *Journal of Chemical Information and Modeling (to appear). Doi:* https://doi.org/10.1021/acs.jcim.1c01065.

Particle flows simulations & particle-particle interactions

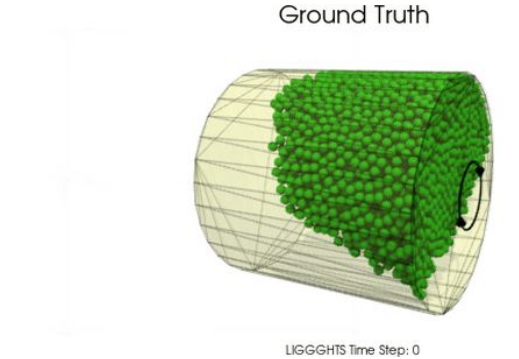
Bad Time Transition Model



Good Time Transition Model



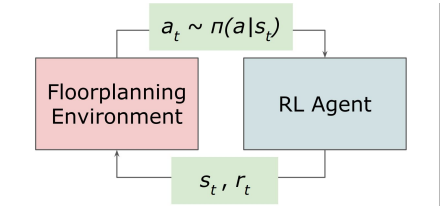
Ground Truth Data

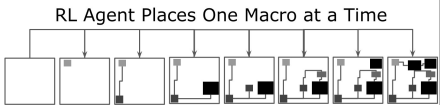


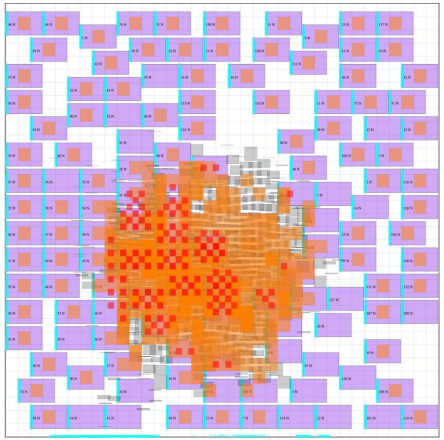
- Prediction of granular flow simulation trajectories by a **deep learning model:** Prediction of acceleration + semi-implicit Euler method to obtain new location
- Machines in industry (hoppers, rotating drums, etc.) described by **triangle meshes** which form **boundaries**
- Boundary Graph Neural Network (**BGNNs**) to learn particle-particle and particle-boundary interactions
- Introduction of an **orientation independent** representation for normal vectors by global ordering

SoC design

- Chip placement: where to place individual components on a given Chip area for optimal performance
- One of the most time consuming stages of SoC design (typically several weeks or months)
- Millions to billions of nodes
- Evaluating one placement through simulation very expensive (e.g. hours to days for one design)
- Train reinforcement learning agent to place components sequentially using proxy reward signal
- Good placement for new SoC within several hours



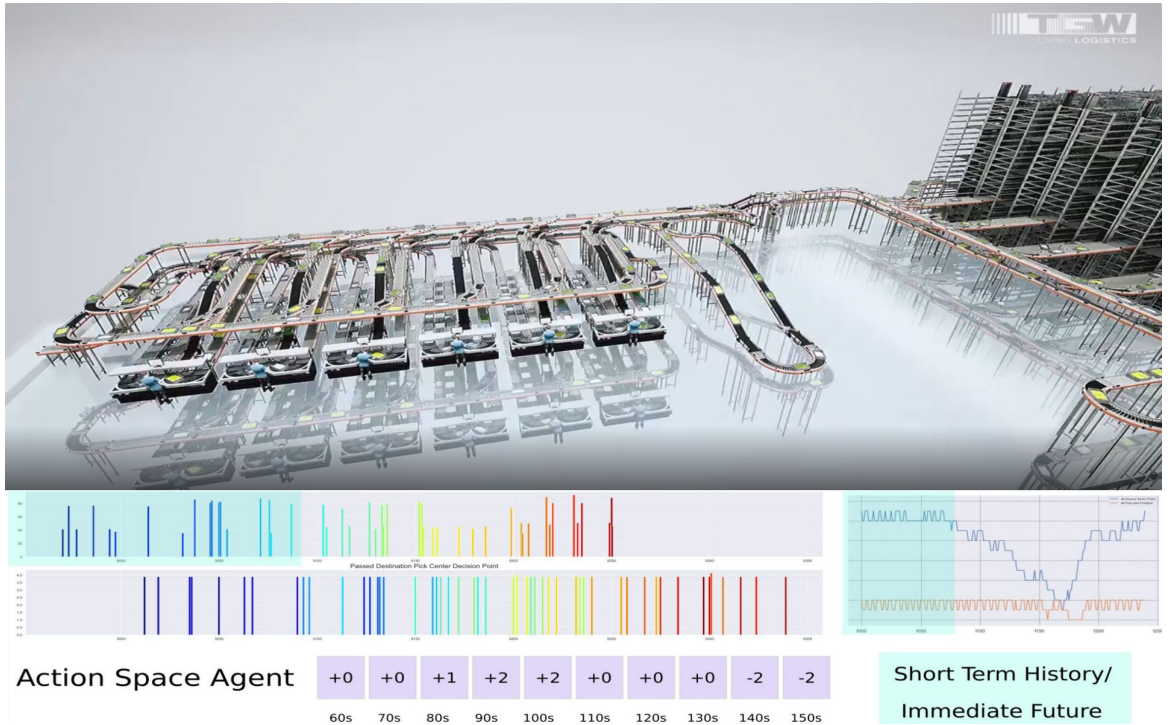




A. Mirhoseini *et al.*, 'A graph placement methodology for fast chip design', *Nature*, vol. 594, no. 7862, pp. 207–212, Jun. 2021, doi: 10.1038/s41586-021-03544-w.

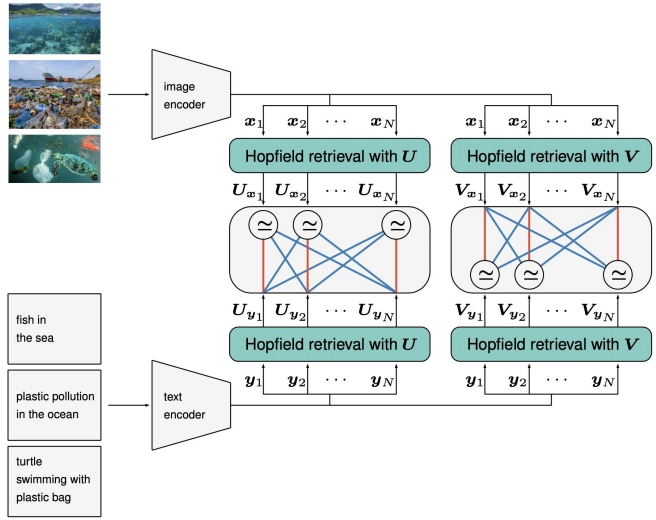
Logistics: resilient warehouse

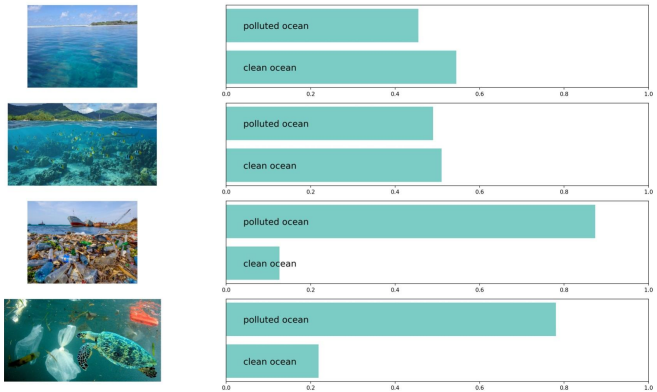
- Use ML to solve a demand and supply problem
- DL for autonomous task scheduling
- Action planning using Reinforcement Learning methods
- Generate optimal lift cycles



CLOOB: connecting text and images

- Novel state of the art self-supervised multimodal learning method
- Hopfield networks (associative memory) used for boosting contrastive learning
- NN pre-trained on a variety of images with a wide variety of NLP supervision
- Use CLOOB as a zero-shot performer
- CLOOB consistently outperforms CLIP across all different downstream tasks for zero-shot transfer learning.





Fürst, A., Rumetshofer, E., Tran, V., Ramsauer, H., Tang, F., Lehner, J., ... & Hochreiter, S. (2021). CLOOB: Modern Hopfield Networks with InfoLOOB Outperform CLIP. *arXiv preprint arXiv:2110.11316*.

Topics of Research

- Deep Learning
- Generative Models (GANs, VAE)
- Reinforcement Learning
- Transformers
- Modern Hopfield Networks
- Few-Shot Learning
- Meta-Learning

- Climate / Earth Science
- Planetary Science
- Physics: Classical & Quantum
- Autonomous Driving
- Drug Discovery / Life Science
- Industrial Applications
- Manufacturing
- Signal Processing (SAL)
- Chip Design (SAL)
- Certification of ML (TÜV)

THANK YOU

Questions?

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