

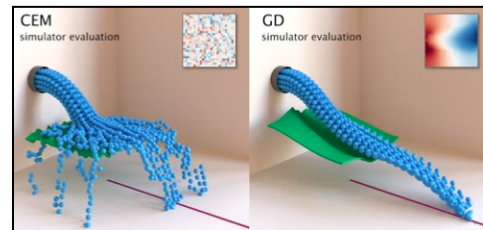
Deep Learning for the Sciences

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MLS: Machine Learning for Simulation Science

Deep learning has been successfully applied in a wide range of use cases and specifically in applications involving visual and textual data. Modern machine translation systems and search engines, for example, are using language models trained on large text corpora.



Increasingly, deep learning is also applied to problems arising in the sciences and engineering. For instance, deep learning for graphs is used to learn simulators from data. The figure on the right shows a particle simulation obtained from a graph neural network trained on simulation traces from a numerical solver. The advantage of using deep learning in this context is its ability to integrate the simulation into a larger neural network with a corresponding loss function and train the resulting model end-to-end.

Other applications of deep learning can be found in chemistry, the biomedical sciences, drug discovery, and engineering disciplines, where use cases range from drug-protein interaction prediction to modeling fluid dynamics. Since machine learning and specifically deep learning will be increasingly used in disciplines of science and engineering, this seminar's goal is to provide an overview of applications, to give students a deeper understanding of recent work, and to have an opportunity to learn how to read, analyze, and engage with scientific papers.

Target group

Participants of the seminar are expected to have completed the course "Machine Learning", "Reinforcement Learning", and/or related courses.

Organization

Students of the *English-speaking* seminar are encouraged to select their own presentation topic, typically based on 1-2 papers and/or a blog post. Alternatively, students can choose from a list of pre-selected topics. In addition to presenting the concrete application of DL, the student will give a brief introduction to the deep learning method used in the paper. Students will give *English* presentations in the weekly seminar. 2 weeks before the presentation, the structure of their presentations will be discussed with the lecturers. After the presentations and before the end of the summer term, the seminar reports must be handed in. Reports are written as **blog posts** and if the students agree, can be published. The seminar is organized by Mathias Niepert who has extensive experience developing (deep) machine learning methods and applying these methods to problems from the biomedical and medical sciences.