High-Performance Computing Group
Prof. Dr. Christian Plessl
Computer Science Department and
Paderborn Center for Parallel Computing

Machine Learning for Electron-Repulsion Integrals

Master Thesis

At a glance

- *No chemistry knowledge is needed.*
- *The calculation of electron repulsion integrals are an important part of quantum chemistry calculations. With traditional algorithms they are very time consuming.*
- *train a neural network to calculate the electron repulsion integrals*

Electron repulsion integrals are a crucial ingredient for many quantum chemistry calculations, like hybrid functional calculations. They are essentially a function from a small set of parameters:

- 4 integer values a, b,c, and d,
- 4 positions in space A, B,C, and D,
- 4 real numbers

to a large set of real numbers. There exist several highly optimized libraries that calculate this function but this calculation is very time consuming. Thus, we expect that applying machine learning to this relation to be beneficial. Reference data for training is easily available.

As the electron repulsion integrals can be viewed as a function, no chemistry knowledge is required for this project. However, a strong background in machine learning techniques is crucial.

Further reading:
available on request

Contact:
Robert Schade, E-Mail: robert.schade@uni-paderborn.de