

Network modularity optimization for maximizing matrix sparsity in large scale quantum chemistry applications

$$S_{ij} = \int_{\mathbb{R}^3} \phi_i(r)\phi_j(r)dr \quad Z^T S Z = 1. \quad F_{\perp} = Z^T F Z$$

How to choose Z in order to maximize sparsity in F_{\perp} ?

- Matrix sparsity important in linear scaling Hartree-Fock (HF) and Density Functional Theory (DFT) calculations.
- Planned master thesis project: explore ways of constructing the inverse factor Z of the overlap matrix, to get as much sparsity as possible.
- Can be done by *network modularity optimization*.

Contact: Elias Rudberg, elias.rudberg@it.uu.se and Emanuel Rubensson, emanuel.rubensson@it.uu.se.