Questions for Carlos

MARTINI Force field: coarse grained model for biomol ecular simulations

* What is an inverted Monte Carlo scheme?

*Monte Carlo:* Their essential idea is using [randomness](https://en.wikipedia.org/wiki/Randomness) to solve problems that might be deterministic in principle. They are often used in [physical](https://en.wikipedia.org/wiki/Physics) and [mathematical](https://en.wikipedia.org/wiki/Mathematics) problems and are most useful when it is difficult or impossible to use other approaches. Monte Carlo methods are mainly used in three problem classes:[[1]](https://en.wikipedia.org/wiki/Monte_Carlo_method#cite_note-1) [optimization](https://en.wikipedia.org/wiki/Optimization), [numerical integration](https://en.wikipedia.org/wiki/Numerical_integration), and generating draws from a [probability distribution](https://en.wikipedia.org/wiki/Probability_distribution). (Wikipedia)

MARTINI Force field: extension to proteins.

Molecular modelling

* What is meant by cut-offs? They work for rapidly decaying bonds, but not for Coulomb interactions? P. 18
* What are Fourier transfroms? How does it work in the PME?
* How does PME work?
* What does the steepest decent in energy minimization mean?
* Neighborlist generation, what does it mean? How does it work?