



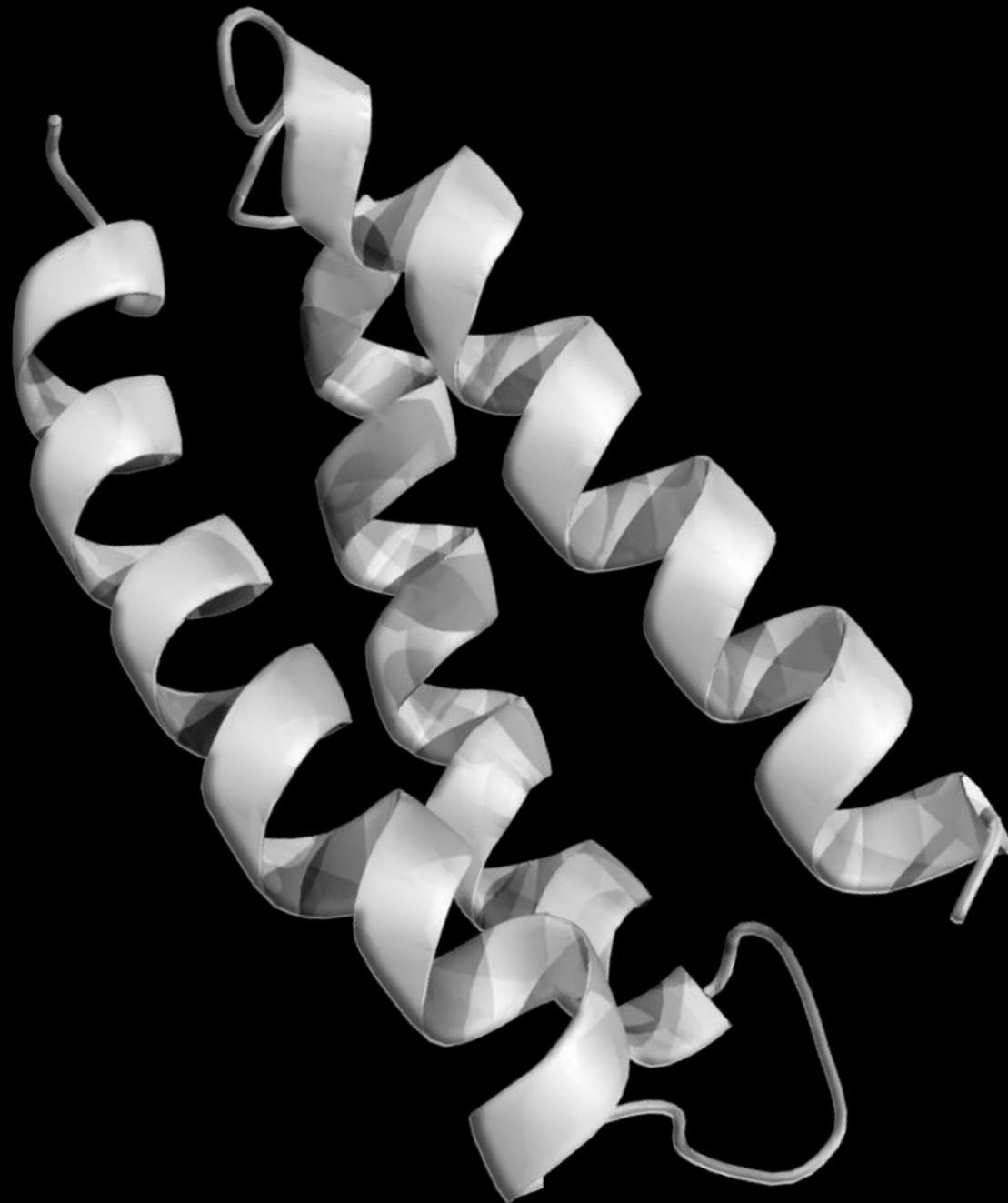
ProtoSyn

Computational design of peptides

Laboratório de Visualização e Computação Científica
Module 2

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Program



Last challenge

30 min

Intro

30 min

Practical examples

30 min

Challenge

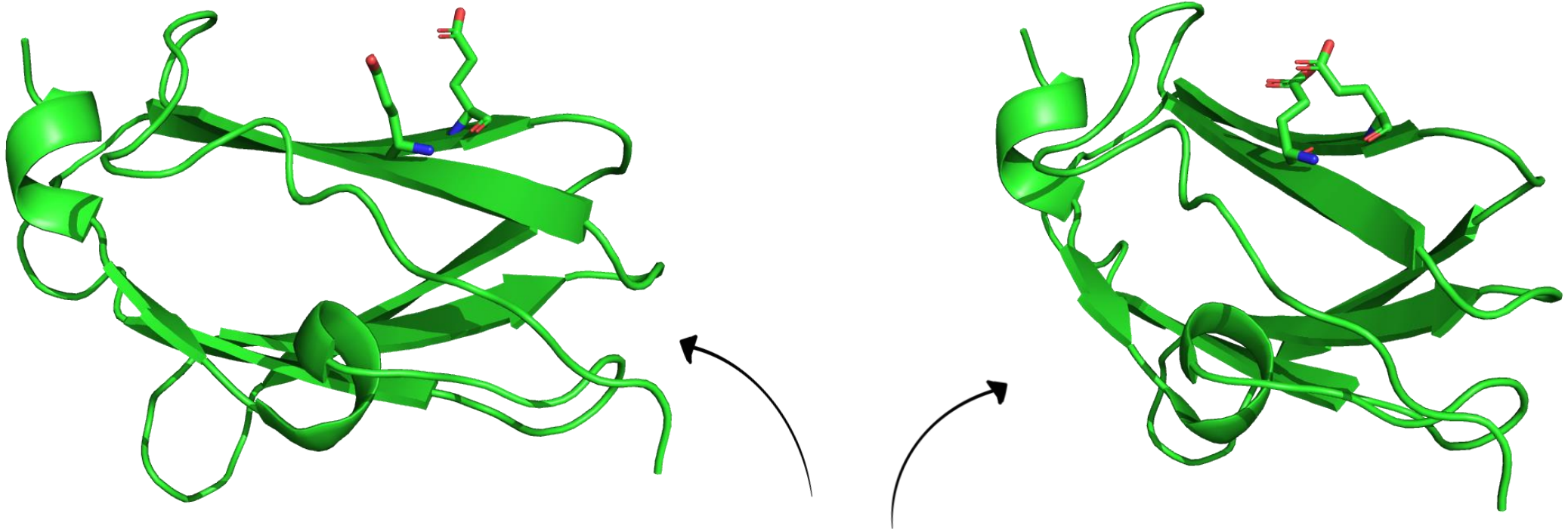
90 min

Break

What's an energy function?

Energy functions measure the energy of a structure.

Less energy = more stable.



Which of these rotamer combinations is more stable?

What's an energy function?

There are many different types of energy functions.

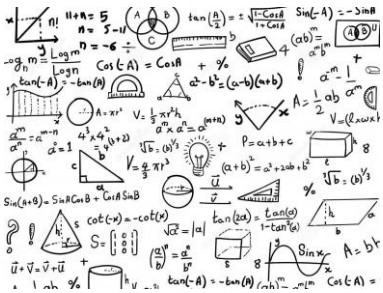
They can be divided based on the **measured components**:

Physical functions

Measure the actual bond distances, angles, deformities and clashes, among others, attributing a reward/penalty based on a set of rules.

Statistical functions

Measure the likelihood of certain characteristics being real, based on big databases collected from real measurements and experiments.



What's an energy function?

There are many different types of energy functions.
They can be divided based on the **level of detail**:

Less accuracy
Faster

More accurate
Slower

Forcefields

A set of simple functions parametrize where atoms should be in relationship to each other.

DFT

Density Function Theory uses quantum physics to calculate the probable positions of electrons, thus inferring all the characteristics that compose a structure (bonds, angles, etc.)

What's an energy function?

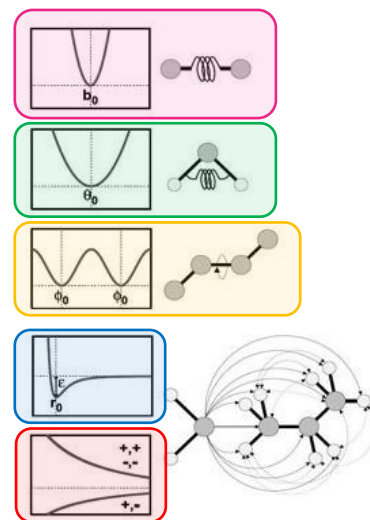
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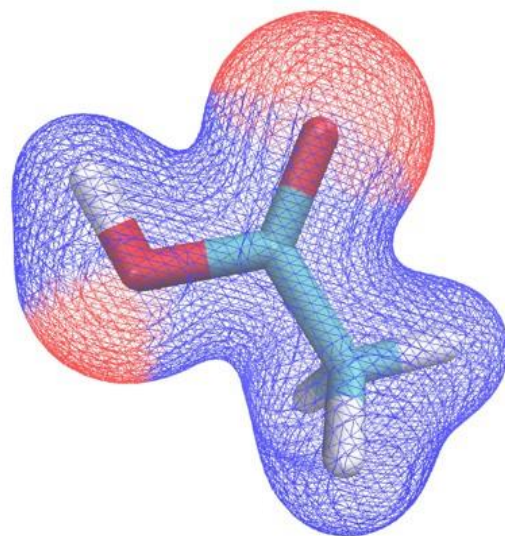
$$E^{\text{MM}} = \sum_{\text{bonds}} K_r (r - r_{\text{eq}})^2 + \sum_{\text{angles}} K_\theta (\theta - \theta_{\text{eq}})^2$$
$$+ \sum_{\text{torsions}} \sum_{n=0}^5 C_n (\cos(\psi))^n + \sum_{\text{impropers}} k_d (1 + \cos(n_d \omega - \omega_d))$$
$$+ \sum_{i>j}^N \left[4\epsilon_{ij} \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] + \frac{1}{4\pi\epsilon_0} \frac{q_i q_j}{r_{ij}}$$

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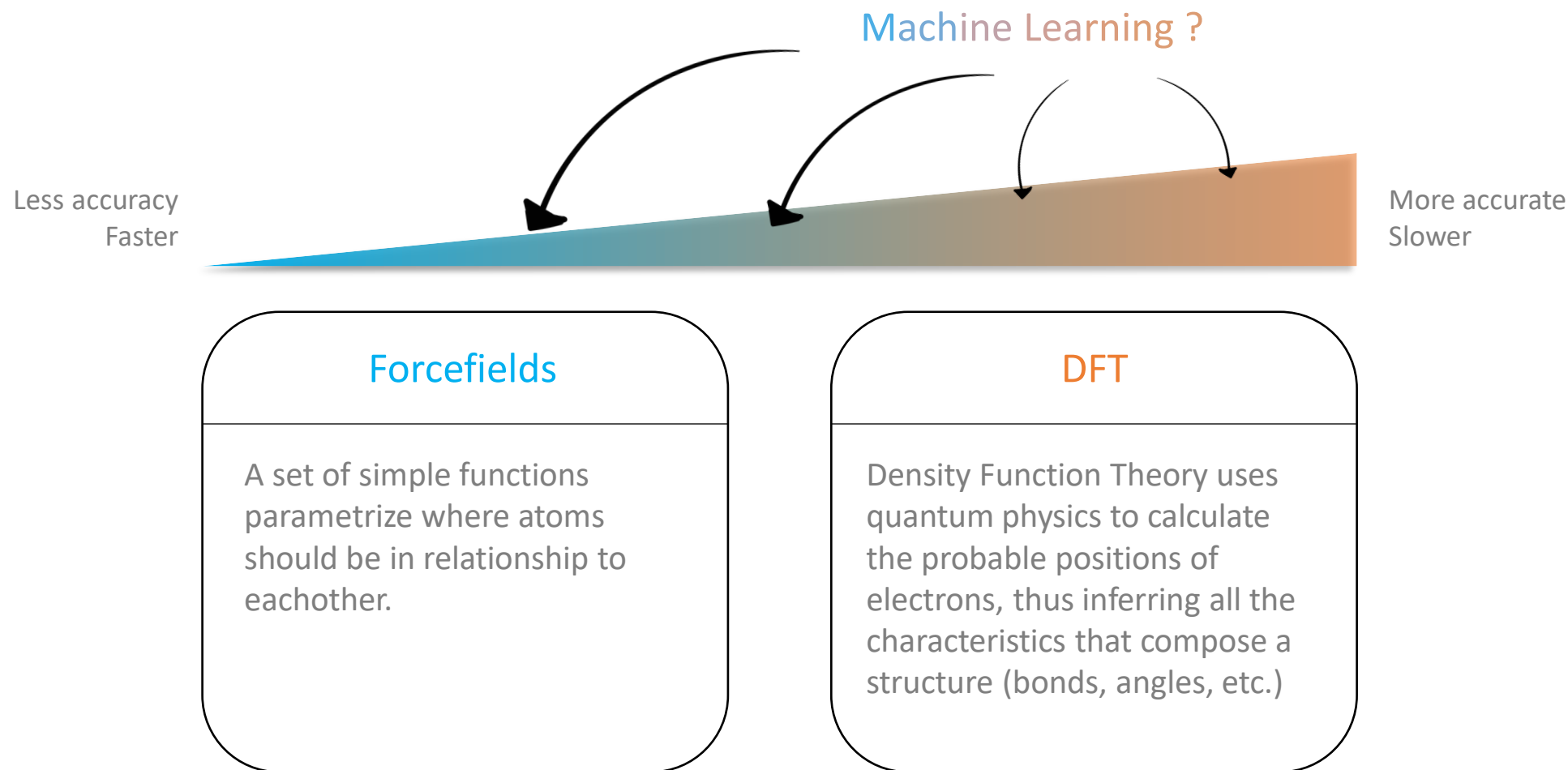
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DFT

Density Function Theory uses quantum physics to calculate the probable positions of electrons, thus inferring all the characteristics that compose a structure (bonds, angles, etc.)

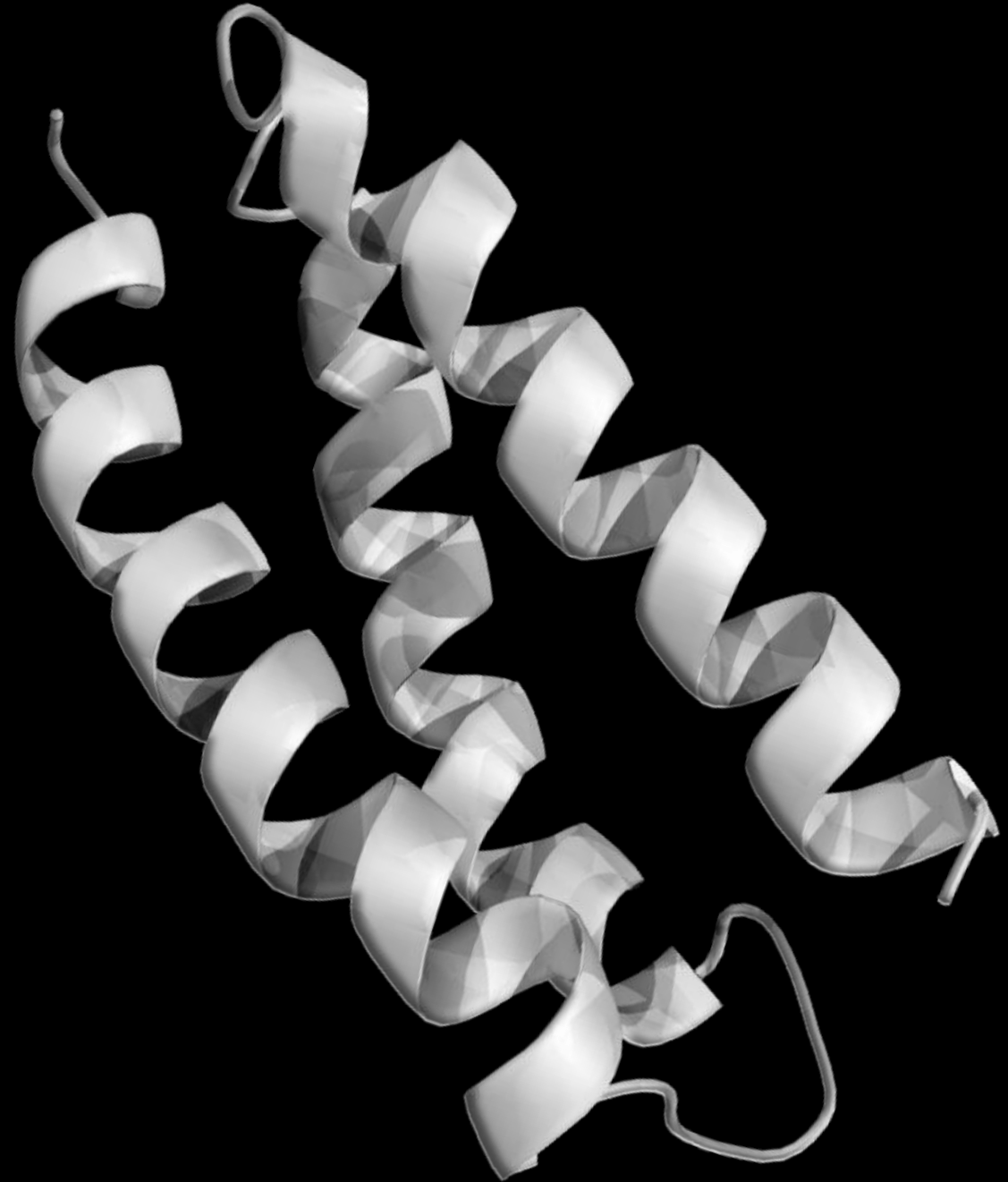
What's an energy function?



Ok ...

Energy functions can calculate how stable a structure is based on a **set of physical rules** or on **how likely those characteristics are to be found in databases**.

There are two major types of energy functions: **forcefields** use simple equations while **DFT** uses quantum chemistry.



The challenge

TorchANI was developed by *Gao et al.*

It's a machine learning model trained on DFT-level solutions.

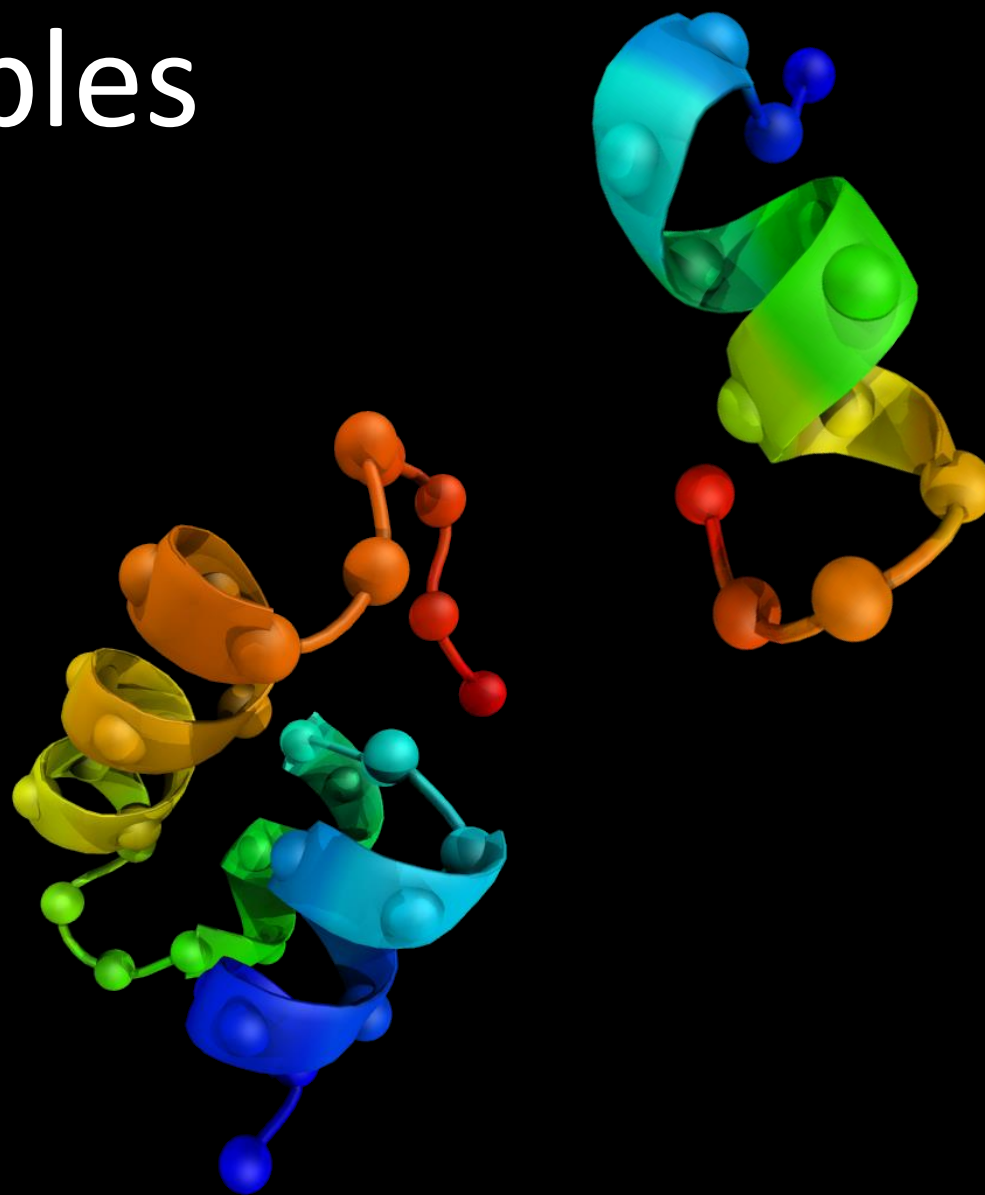


<https://github.com/aiqm/torchani>

[An example](#)

Some practical examples

1. Measure the energy of a molecule



The challenge

1. Develop a Monte Carlo simulation in order to pack the sidechains of a Molecule

