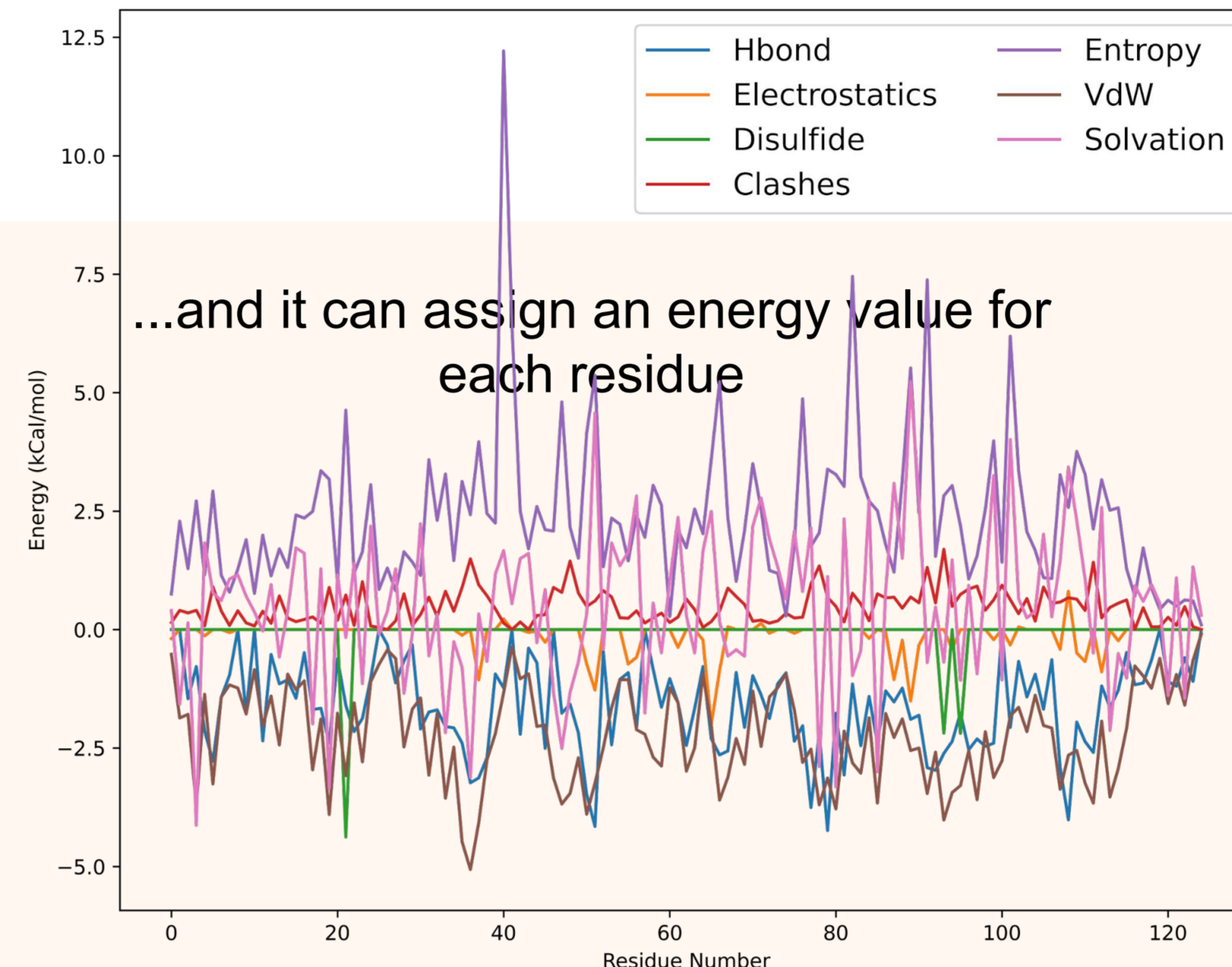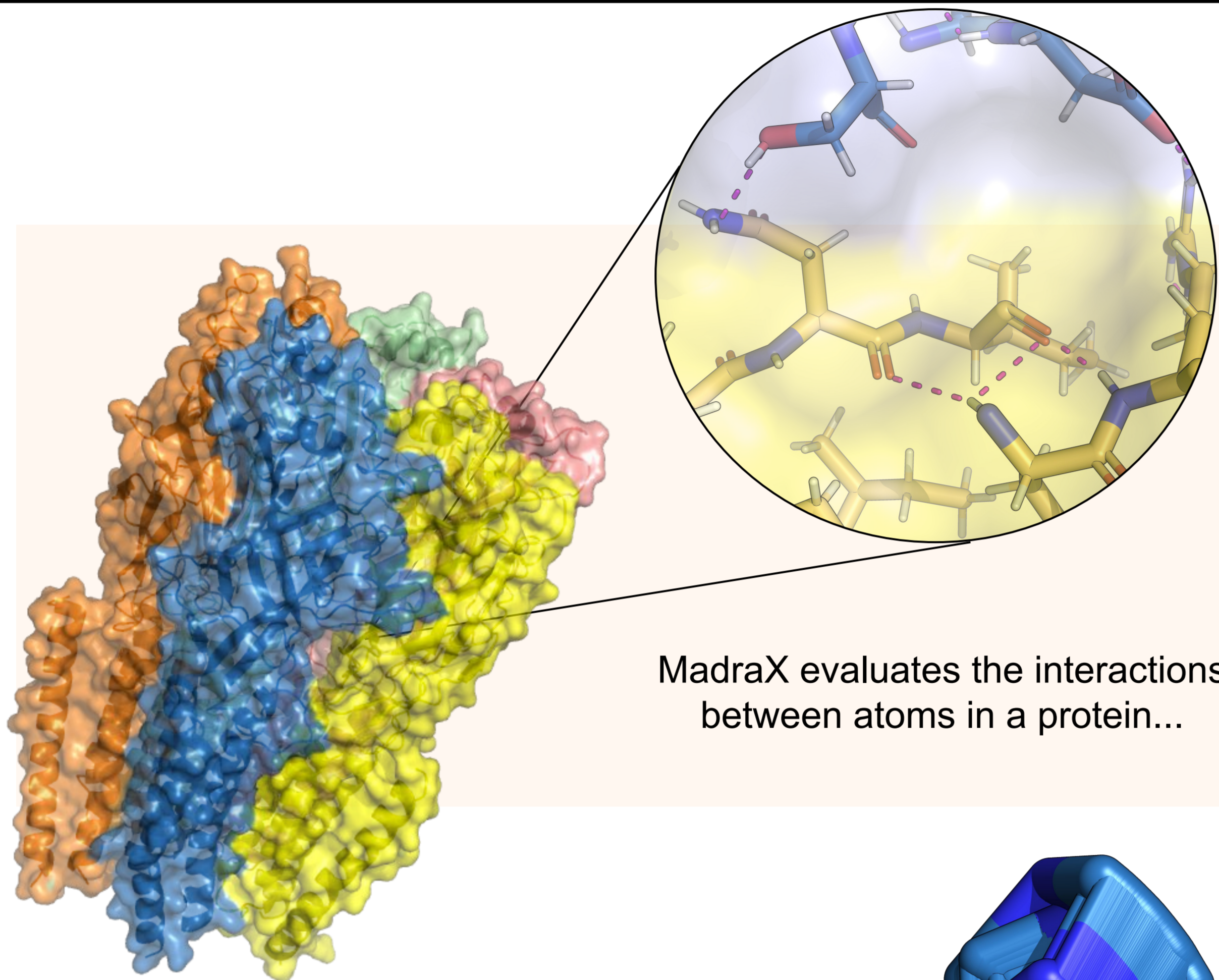# Inclusion of physical models in artificial neural networks
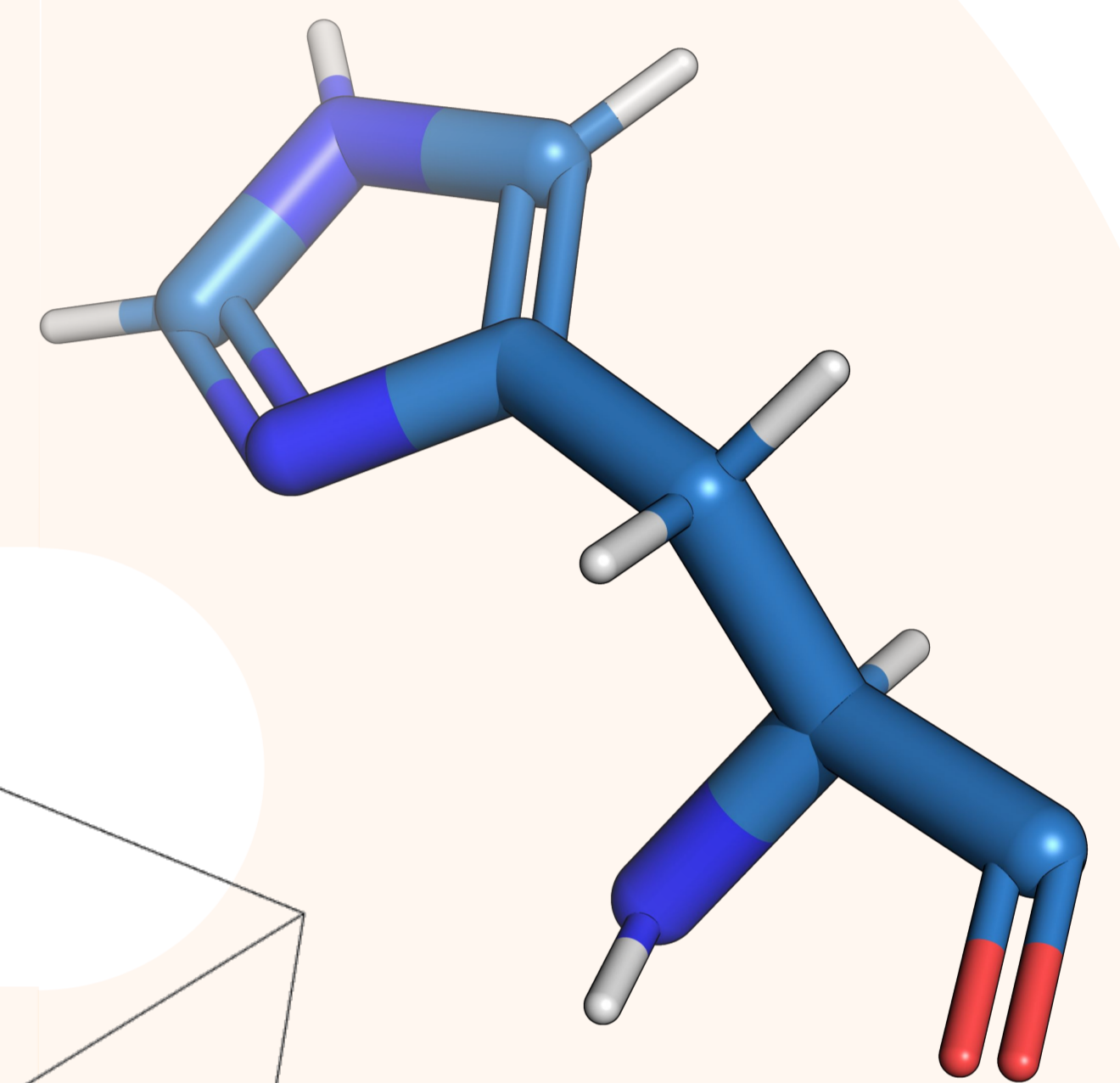
Gabriele Orlando

Laboratory of Pathogens and Host Immunity (LPHI)

Background
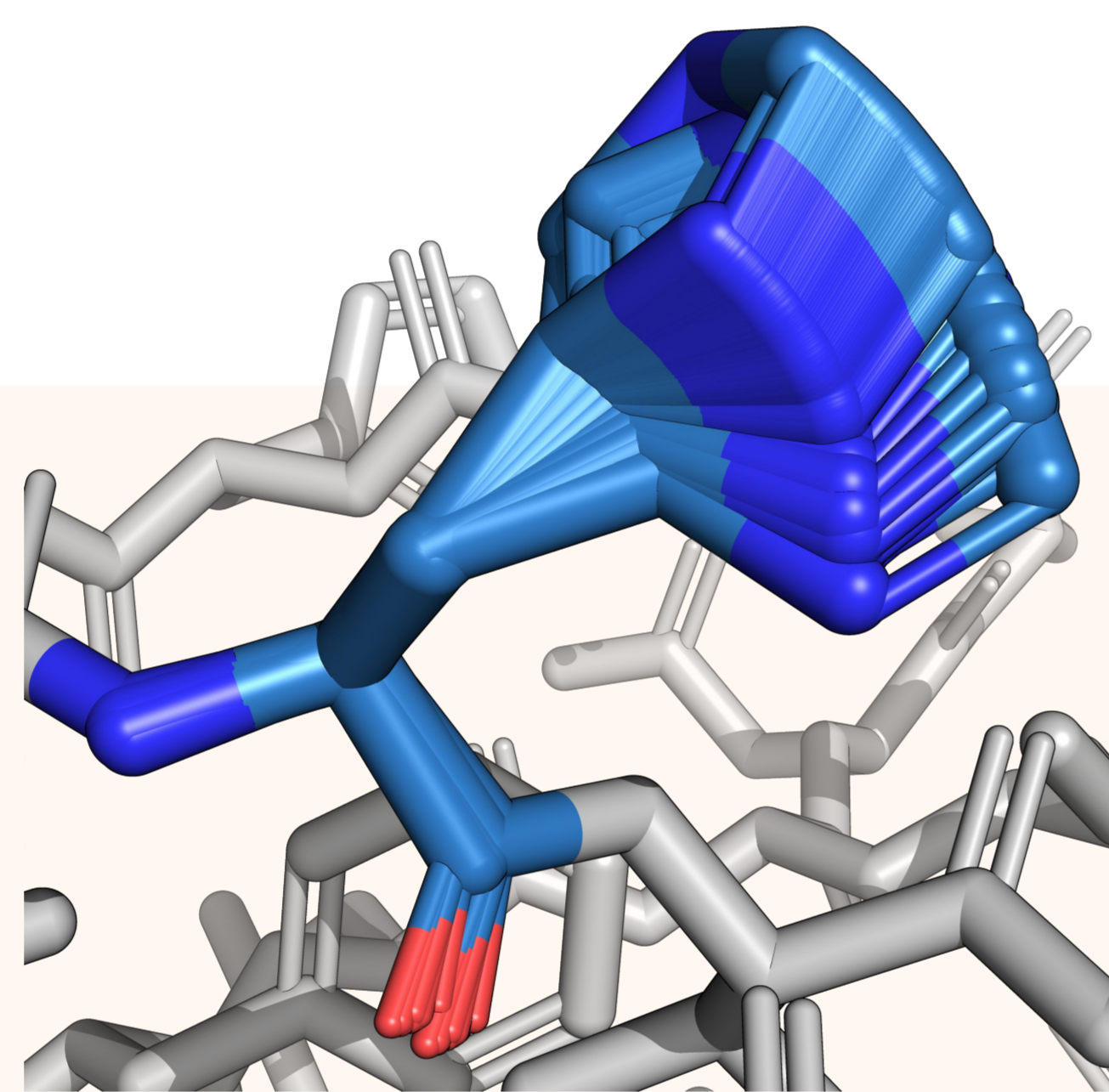
1) A force field is a set of physical rules that describe the interaction forces between atoms.
2) A coding language that supports automatic differentiation (i.e. PyTorch) can compute gradients of functions automatically, without manual derivation.
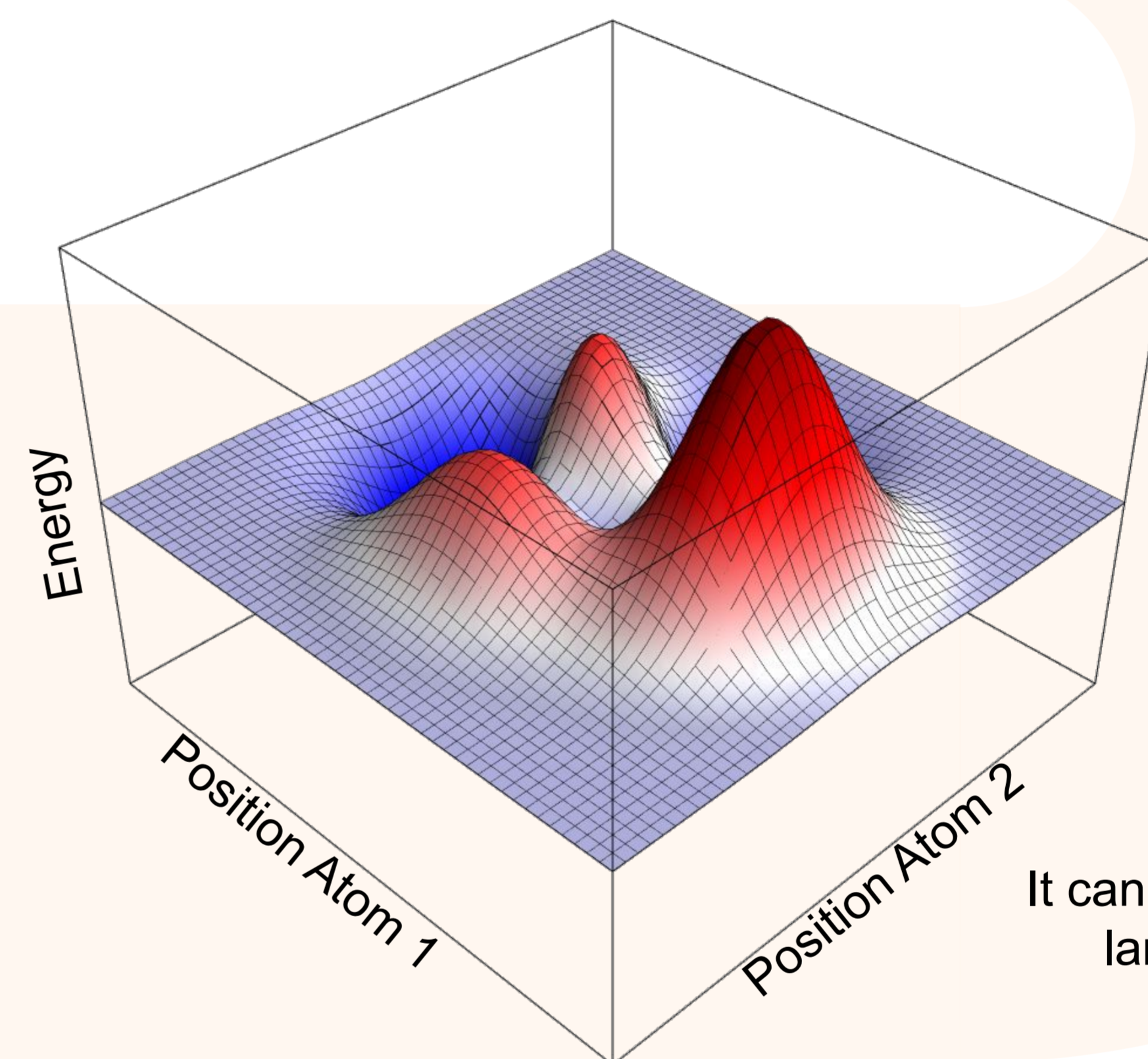3) We developed MadraX, a force field for proteins that allows automatic differentiation.

MadraX evaluates the interactions between atoms in a protein...

...and it can assign an energy value for each residue

It can use the automatic differentiation to calculate the gradient of the energy with respect to atom positions.
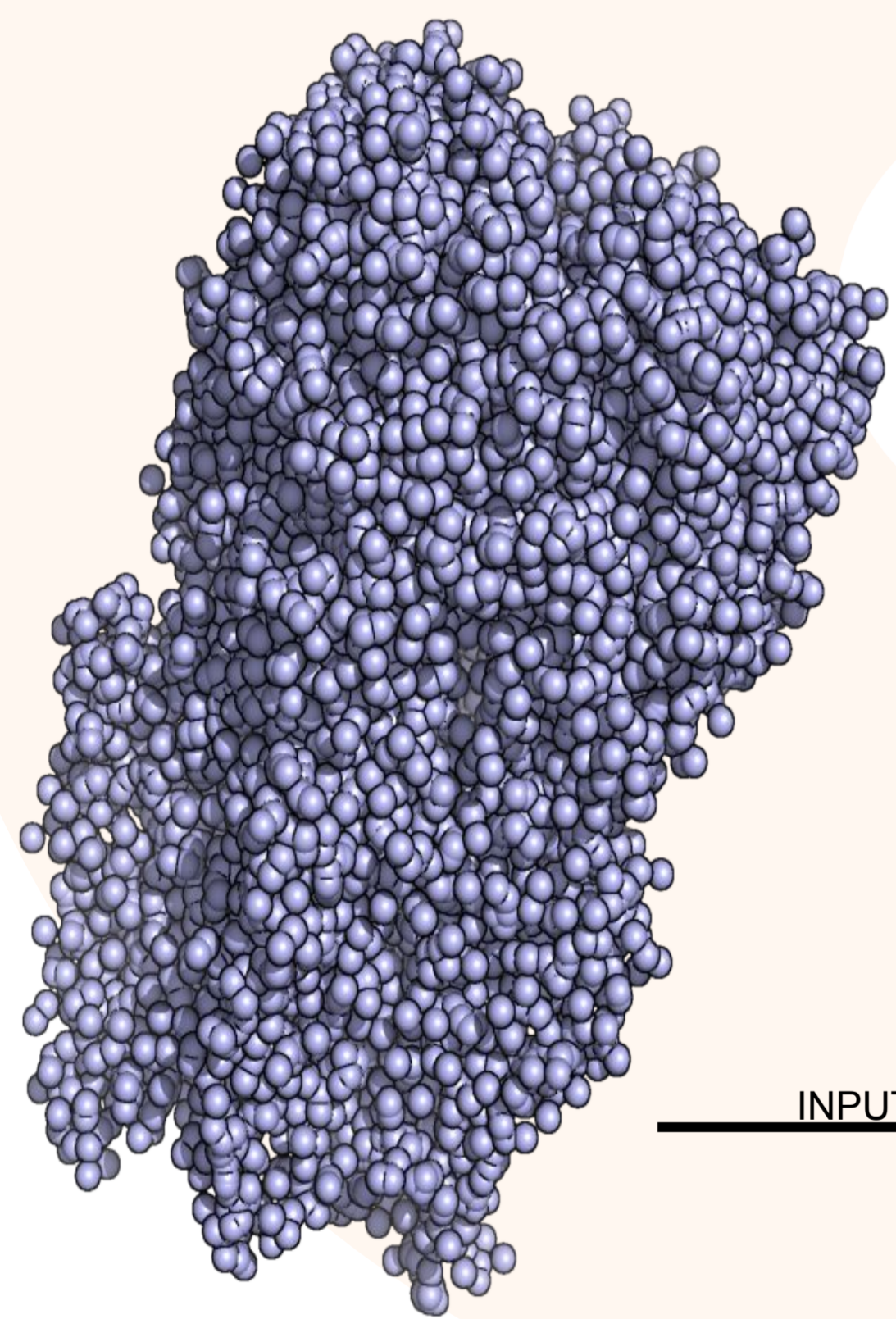
pyUUL

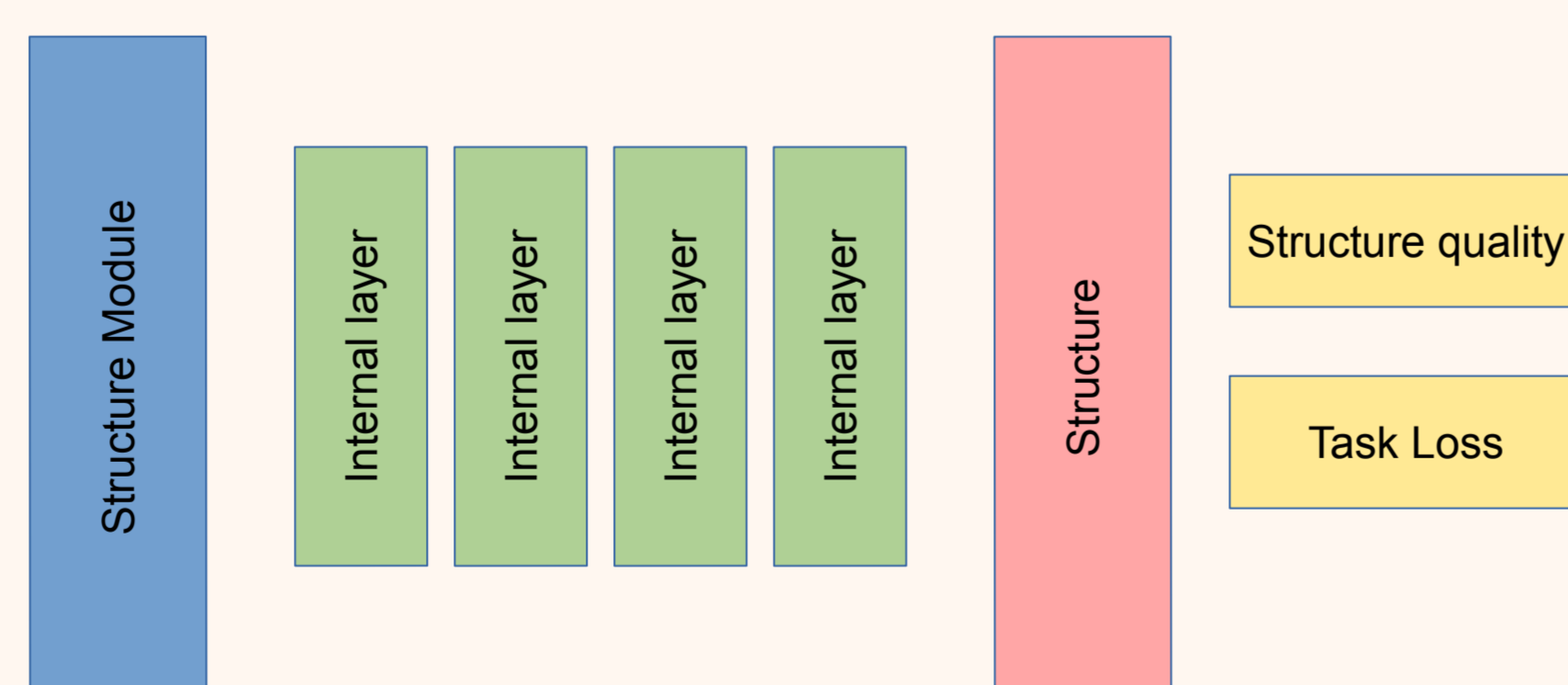To convert protein structures in a format that neural networks can handle

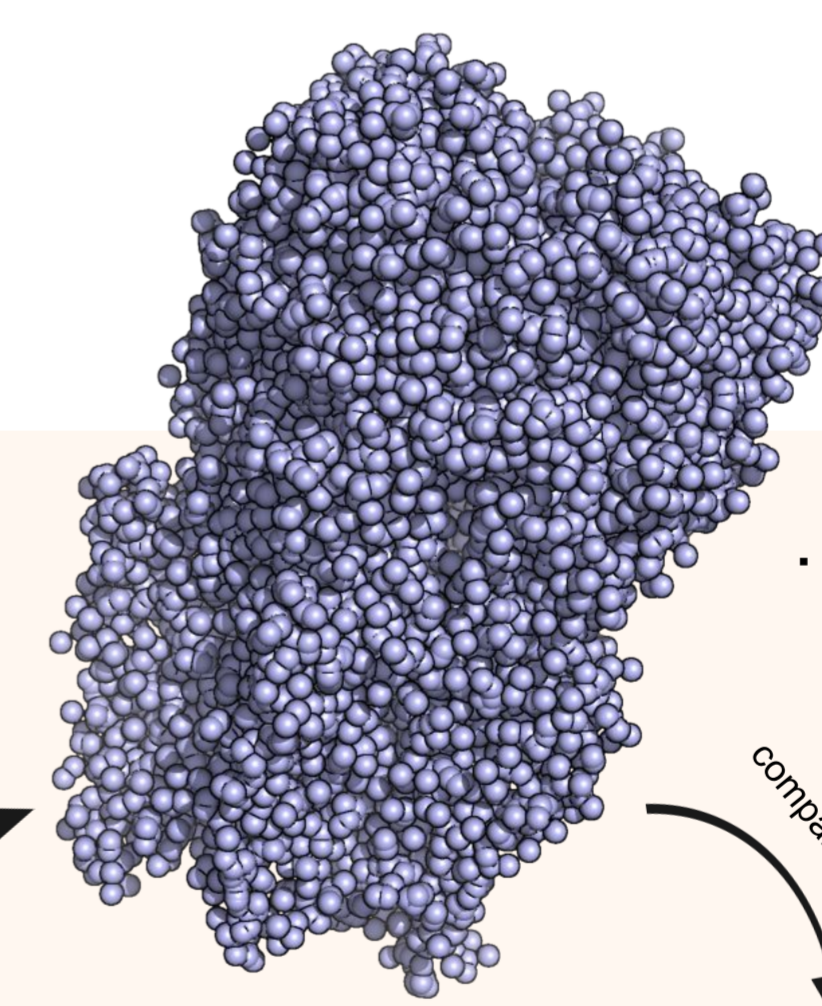...and tell where an atom should move to to minimize its energy

It can therefore define an energy landscape with respect to the atom's position…

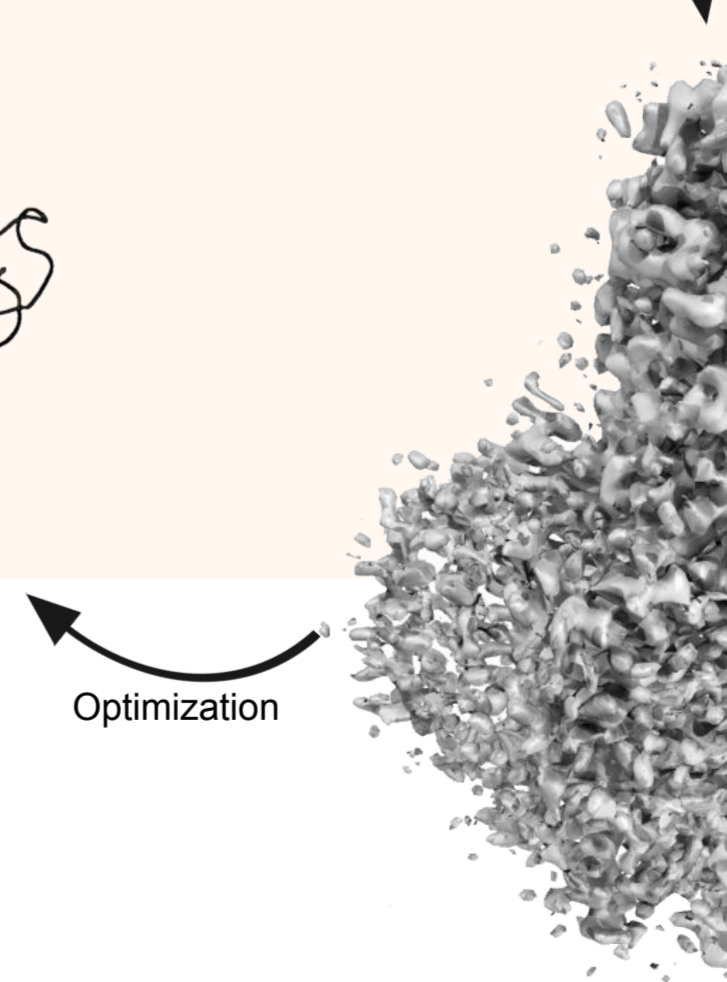Or it can be used inside a neural network that works with protein structures…

…constraining the network to learns only physically sound rules…

…making therefore the network aware of physics.

For example, here you can find a video of a neural network with MadraX optimizing a cryoEM structure

INPUT

Structure Module

Internal layer

Structure

Structure quality

Task Loss

conversion

comparison

Optimization

Objective

Include MadraX into a neural network that is capable of predicting liquid-liquid phase separation.