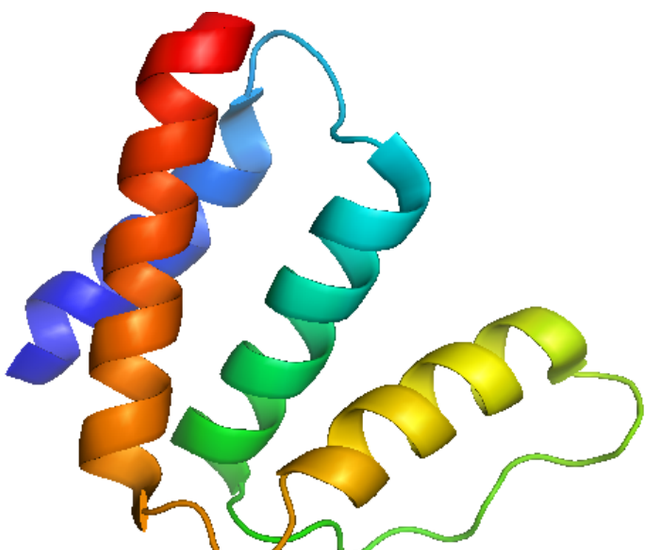
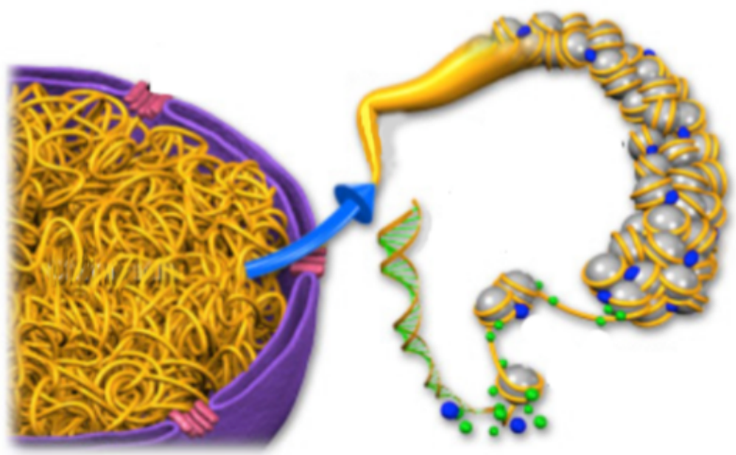
BioPhys - Milano

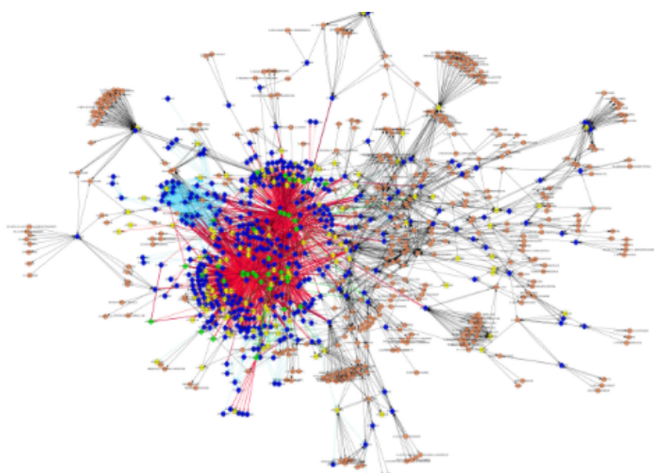
"The main goal of the BioPhys network is the study of problems and systems of Biological interest with the tools and ideas typical of theoretical physics."



Proteins



Chromatin



Genetic networks

Techniques:

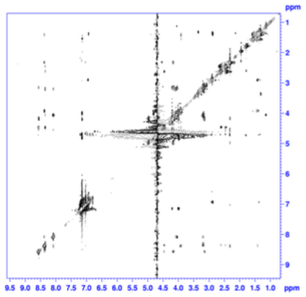
- algorithms for conformational sampling (Monte Carlo, etc.)
- simplified models guided by experimental data (MaxEnt)
- molecular dynamics
- machine learning

- dimensional reduction
- replicas
- inverse statmech models
- differential equations (for genetic networks)

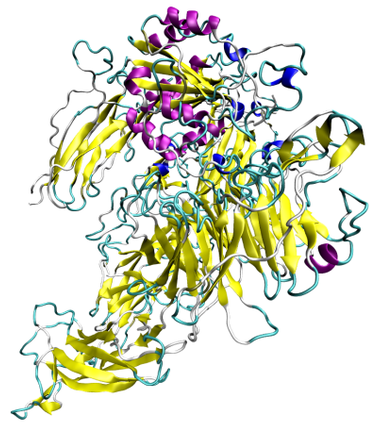
Example 1: reconstruction of protein ensemble from NMR data

Usual procedure (mean field)

Experimental data
(dipolar couplings between ^{1}H or ^{13}C)

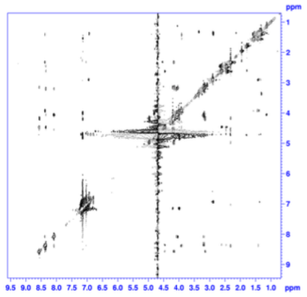


$$I_{ij} = I_0 \left\langle \frac{1}{d_{ij}^6} \right\rangle \approx I_0 \frac{1}{\langle d_{ij} \rangle^6}$$



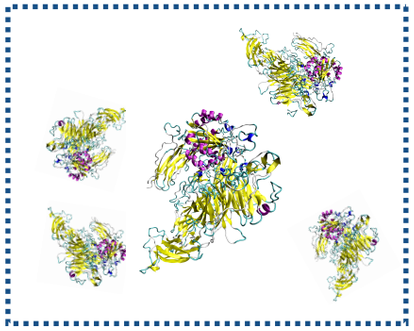
Beyond mean field

Experimental data



+ Approximated potential $U_0(\{r_i\})$

Conformational ensemble

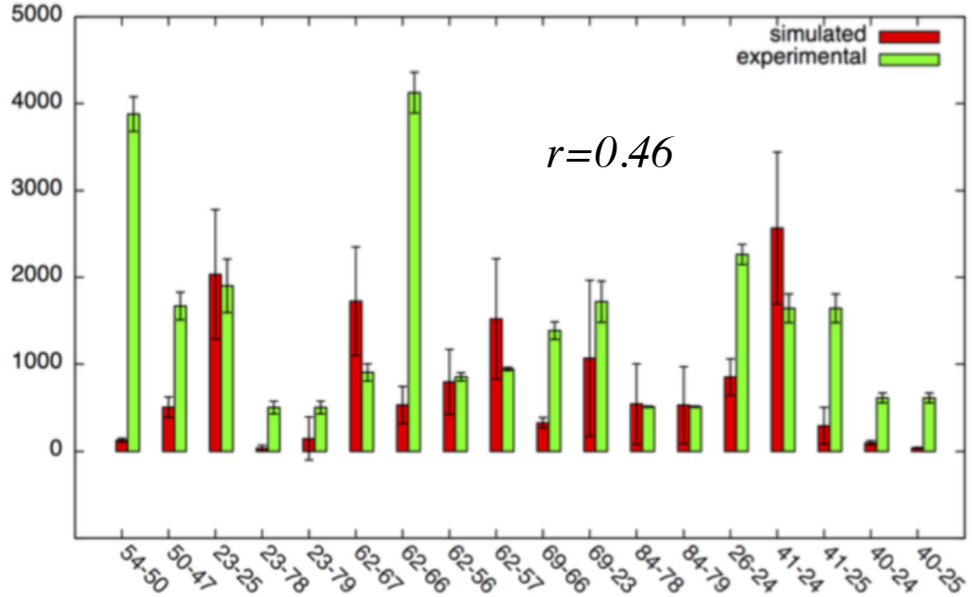


- Principle of maximum entropy $$\frac{\delta}{\delta p(r_i)} \left[-\int dr_i \, p(r_i) \log p(r_i) - \sum_m \lambda_m \left(\int dr_i \, f_m(r_i) p(r_i) - f_m^{exp} \right) - \dots \right] = 0$$

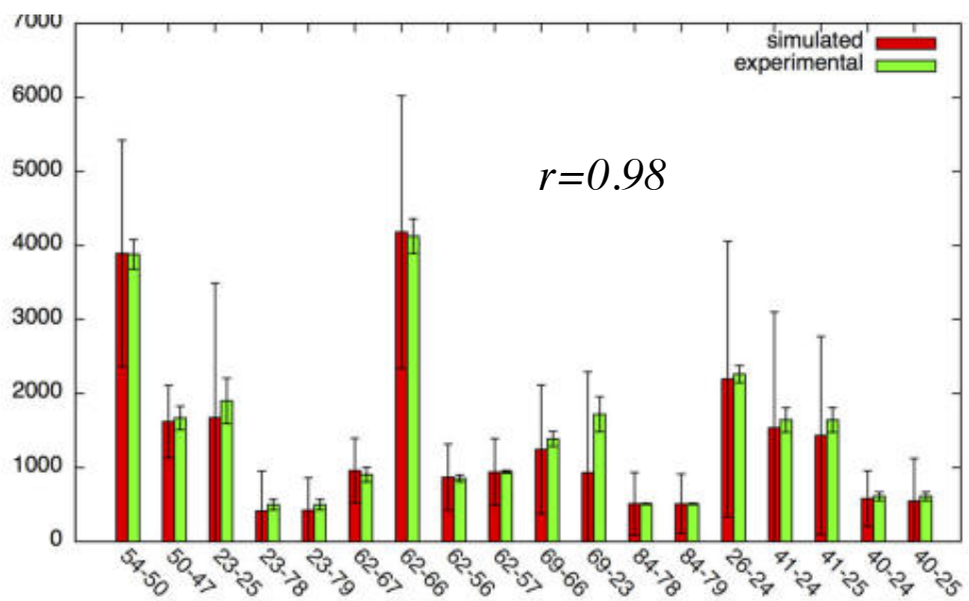
- Less approximated modelling of the data $I_{ij}(\tau_m) = e^{-W\tau_m} I_{ij}(0)$ where $W_{ij} = \overline{\langle i | \hat{H}_{dc} | j \rangle} \sim \frac{1}{d_{ij}^6}$

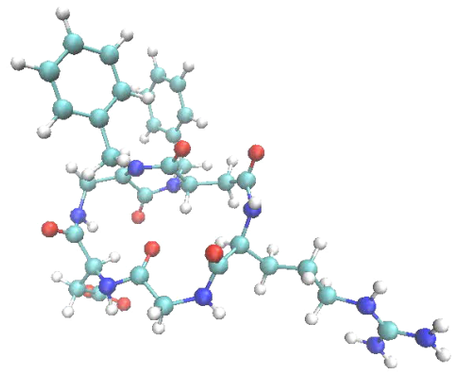
- Iterative Monte Carlo sampling

U_0



U_0 + data-based correction





Example 2: dimensional reduction of protein coordinates using artificial neural networks