Pisa group – Biophys

Activity

The activity of the Pisa group is focused on the developments and applications of numerical simulation methods of complex systems of biological interest.

Members (FTE: 5.0)

Name -- Position -- INFN Position

Giuseppe Brancato – Professore Aggregato RU 100%

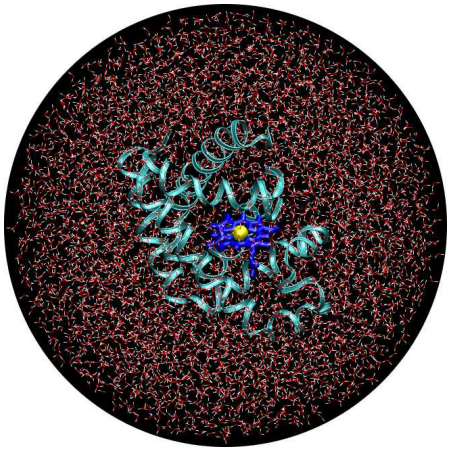
Vincenzo Barone -- Professore Ordinario 100%

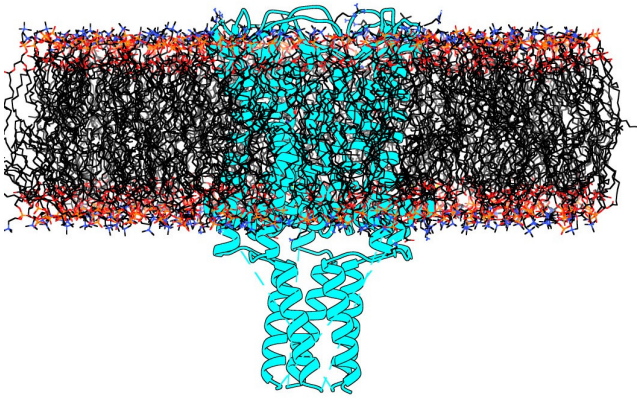
Giordano Mancini -- Tecnico 100%

Sergio Rampino -- Ricercatore Universitario RTDA 100%

Luca Sagresti – Dottorando 100%

Molecular Dynamics (MD) Simulations





Size: >100,000 atoms

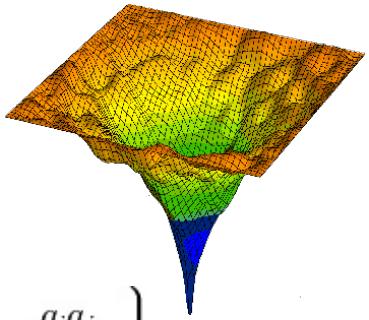
Time scale: 100 ns – 1 μs

Molecular dynamics is a computational method that allows to follow the time evolution of a molecular system on the basis of a known potential

Simulation with full atomistic details:
Protein
Environment (Solvent + Lipid Membrane)

Molecular mechanics force fields

$$V(r^N) = \sum_{\text{bonds}} \frac{1}{2} k_b (l - l_0)^2 + \sum_{\text{angles}} k_a (\theta - \theta_0)^2 + \sum_{\text{torsions}} \frac{1}{2} V_n [1 + \cos(n\omega - \gamma)] + \sum_{j=1}^{N-1} \sum_{i=j+1}^{N} \left\{ \epsilon_{i,j} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - 2 \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right] + \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}} \right\}$$



Richieste 2022

Missioni Interne ed esterne: 7.5KE (5.0 FTE)

1) Prof.sa Annalisa Pastore, King's College, UK
2) Prof.sa Armagan Kocer, Univ. Groeningen, NL
3) Prof. Dario Alfé – University College London, UK

Partecipazione alle seguenti conferenze

1) CECAM Workshop
2) ACS Conferences
3) ESP Conference

Inviti Ospiti Stranieri

Prof. Giovanni Bottari

Universidad Autonoma de Madrid, Spain