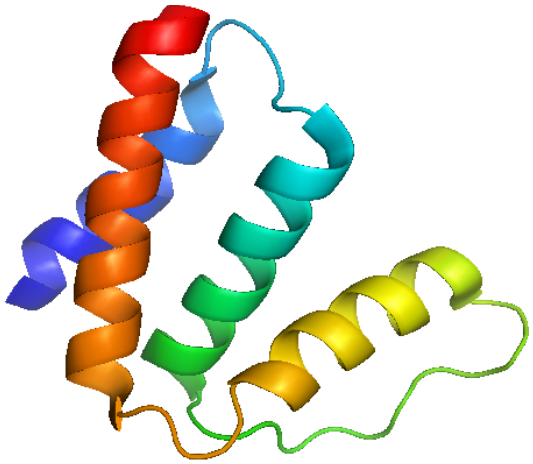
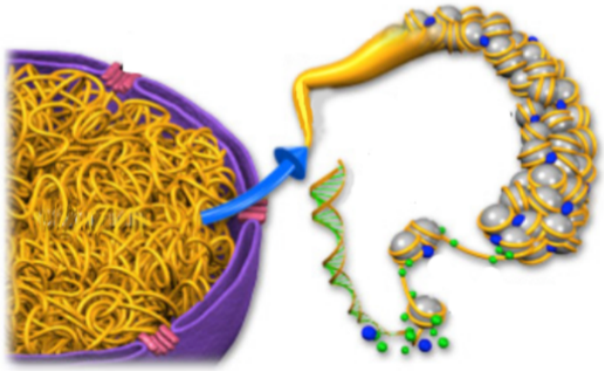
BioPhys - Milano

"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."



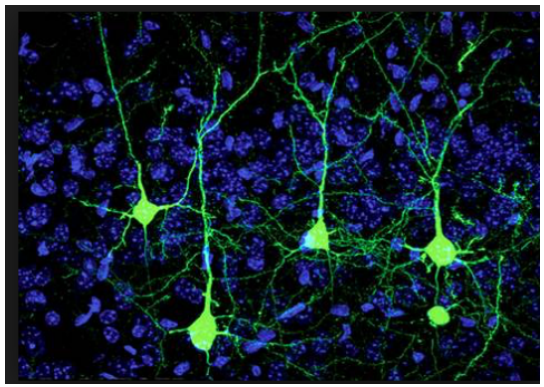
Proteins

with Harvard University, TUM, Dept. Biosciences UNIMI



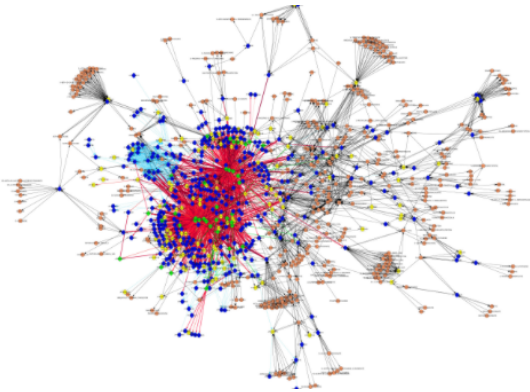
Chromatin

with ENS, Institut Curie, FMI Basel



Neural activity

with UCSD



Genetic networks

with NBI, Zapperi group

Team:

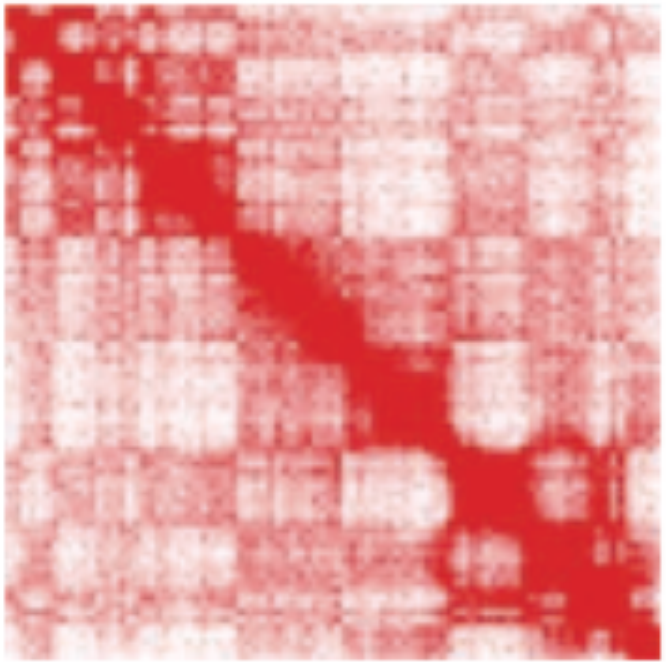
Guido Tiana (PI)
Roberto Meloni, Riccardo Capelli, Filippo Cola (dottorandi)

Techniques:

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

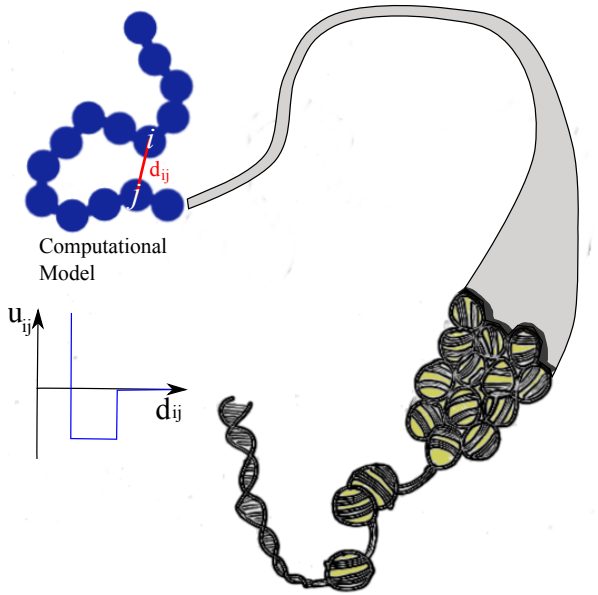
- dimensional reduction
- replicas
- inverse statmech models
- differential equations (for genetic networks)

Example: chromatin



Chr 14

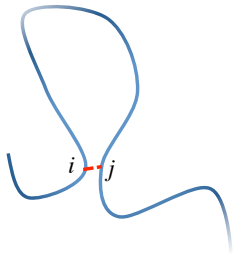
1 Mb resolution



- conformational fluctuations/correlations
- correlation with gene activity
- response (differentiation, disease)

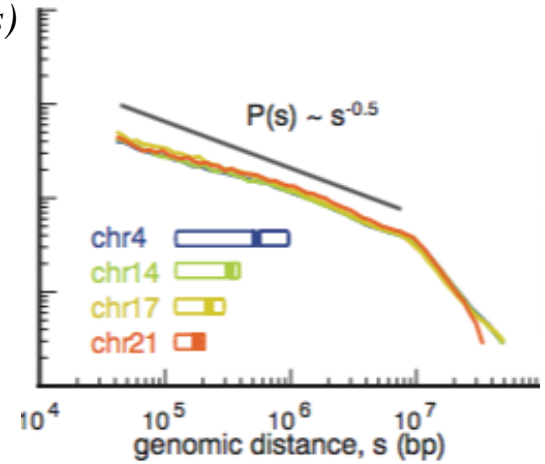
L. Giorgetti *et al.*, Cell 2014

looping probability



$$p_{ij} \sim \frac{1}{|j-i|^{\gamma}} \qquad \gamma = \begin{cases} 3/2 & \text{for ideal chains} \\ 9/5 & \text{for random coils} \\ 0 & \text{for random globules} \end{cases}$$

$P(s)$



$$\overline{Z_{ij}^{n}} = \int d\{r^{\alpha}\}\left(v^{n}\prod_{\alpha}\delta(r_i^{\alpha}-r_j^{\alpha})\right) \times \exp\left[-\beta\sum_{\alpha}U_1(\{r_l^{\alpha}\}) + \frac{\beta^2\sigma^2}{2}v^2 \times \sum_{k\neq l\,\alpha\neq\beta}\delta(r_k^{\alpha}-r_l^{\alpha})\delta(r_k^{\beta}-r_l^{\beta})\right],$$

$$\sum_{k<l}\Big[\underset{k\ l\ i\ j}{\cdot\!\cdot\!\circ\!\circ} + \underset{k\ i\ l\ j}{\cdot\!\circ\!\cdot\!\circ} + \underset{i\ k\ l\ j}{\circ\!\cdot\!\cdot\!\circ} + \underset{i\ j\ k\ l}{\circ\!\circ\!\cdot\!\cdot} + \underset{i\ k\ j\ l}{\circ\!\cdot\!\circ\!\cdot} + \underset{k\ i\ j\ l}{\cdot\!\circ\!\circ\!\cdot}\Big].$$

$$\overline{\log p(\Delta l)} = \ln\left\{\frac{1}{\Delta l^{\kappa}}\exp\left[-\left(\frac{\Delta l}{\Delta l_0}\right)^{2\kappa-2}\right]\right\}$$

G. Tiana, Phys. Rev. E 2015