

IMMAGINI E RIFLESSIONI TESI

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1 GRAFO

Allora la scelta per il grafo, per semplicità di scrittura è stato quello di fare dei legami solo e solo se il raggio di interazione è minore di un certo valore. Come si fa a trovare la threshold migliore per il raggio in questo modello? Si runna il modello al fine di minimizzare i MAE sui residui ogni volta con un raggio diverso. Il modello che ottiene il mae minore è quello che meglio descrive il tutto. Inoltre in questo modo è possibile ottenere anche il miglior grafo senza alcun tipo di vincolo. Prima di predire i beta factor per davvero (con autovalori e autovettori) avrei bisogno di utilizzare i parametri corretti e per temperatura Kb ecc.

2 Matrice di kirchoff

La matrice di Kirchhoff (o laplaciana) rappresenta un'analogia con una rete elastica in cui le connessioni tra i nodi (atomi) descrivono le interazioni elastiche. Questa matrice codifica il modo in cui ogni nodo è collegato agli altri, e attraverso i suoi autovalori e autovettori, si può studiare come le vibrazioni collettive (modi normali) si propagano attraverso il sistema. Autovalori e autovettori della matrice di Kirchhoff: Gli autovalori della matrice di Kirchhoff descrivono le frequenze naturali di vibrazione del sistema. Gli autovettori rappresentano i corrispondenti modi normali di vibrazione, cioè come ogni nodo (atomo) si muove in un determinato modo di vibrazione. Quelli a bassa frequenza corrispondono alle vibrazioni collettive del sistema, quelli ad alta frequenza sono fluttuazioni locali

3 Calcolo correlazione

Risolvi l'equazione differenziale:

$$\gamma \dot{x}_i = -g \sum_j K_{ij} x_j + \sqrt{2\gamma k_B T} \xi_i(t) \quad (1)$$

$$\mathbf{x}(t) = e^{-\mu K t} \left\{ \mathbf{x}(0) + \sqrt{\frac{2k_B T}{\gamma}} \int_0^t ds e^{-\mu K s} \xi(s) \right\} \quad (2)$$

$$C(t) = \langle \mathbf{x}(0) \mathbf{x}^\top(t) \rangle \quad (3)$$

$$C(t) = e^{-\mu \mathbf{K} t} C(0) \quad (4)$$

$$C(0) = \langle \mathbf{x}(0) \mathbf{x}^\top(0) \rangle \quad (5)$$

$$\mathbf{K} = \mathbf{U} \Lambda \mathbf{U}^\dagger \quad (6)$$

$$C_{ij}(t) = \frac{3k_B T}{g} \sum_{k=2}^N \frac{u_i(k) u_j(k)}{\lambda(k)} e^{-\lambda(k)t} \quad (7)$$

4 Calcolo risposta

$$R(t) = \frac{C(t)}{C(0)} \quad (8)$$

$$\mathbf{R}(t) = e^{-\mu \mathbf{K} t} \quad (9)$$

$$R_{ij}(t) = - \left\langle \frac{\partial \ln P_s(x)}{\partial x_j(t)} x_i(0) \right\rangle \quad (10)$$

$$R_{ij}(t) = \sum_{k=1}^N u_i(k) u_j(k) e^{-\lambda(k)t} \quad (11)$$

5 Cross-Entropy

$$TE_{j \rightarrow i}(t) = \left\langle \log \frac{P[x_i(t)|x_i(0), x_j(0)]}{P[x_i(t)|x_i(0)]} \right\rangle \quad (12)$$

$$T_{j \rightarrow i}(t) = -\frac{1}{2} \ln \left(1 - \frac{\alpha_{ij}(t)}{\beta_{ij}(t)} \right) \quad (13)$$

$$\alpha_{ij}(t) = [C_{ii}(0)C_{ij}(t) - C_{ij}(0)C_{ii}(t)]^2 \quad (14)$$

6 2M0Z

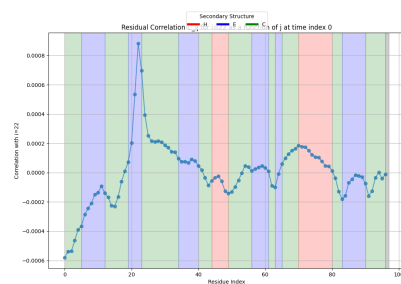


Figure 1: Correlazione

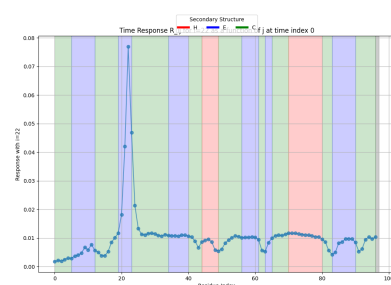


Figure 2: Risposta

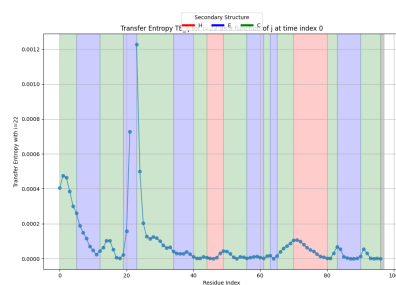


Figure 3: Transfer Entropy

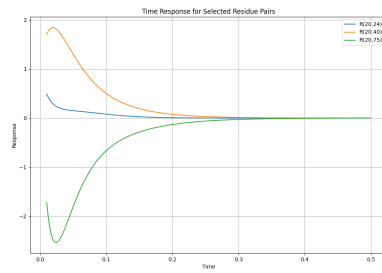


Figure 4: Multiple time response

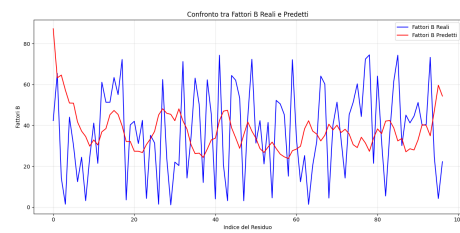


Figure 5: B factors

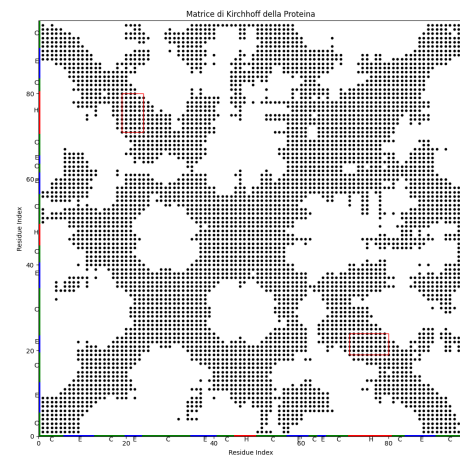


Figure 6: Kirchhoff

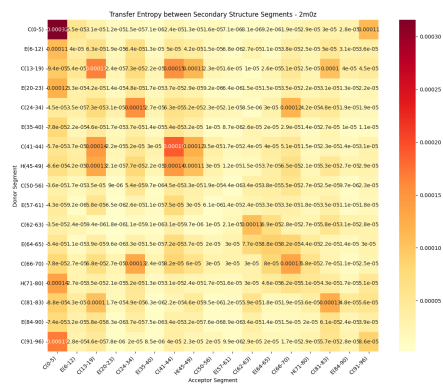


Figure 7: Secodnaria Structure

7 2M10

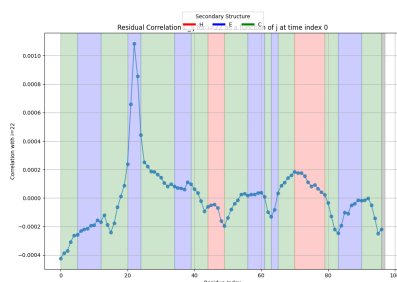


Figure 8: Correlazione

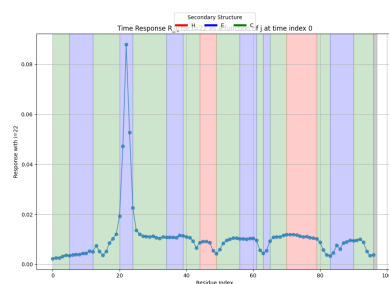


Figure 9: Risposta

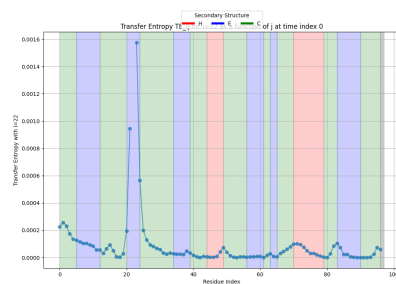


Figure 10: Transfer Entropy

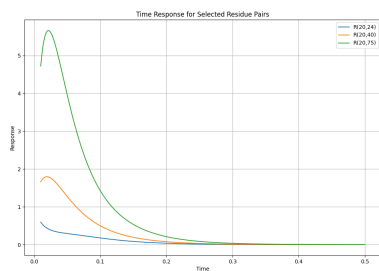


Figure 11: Multiple time response

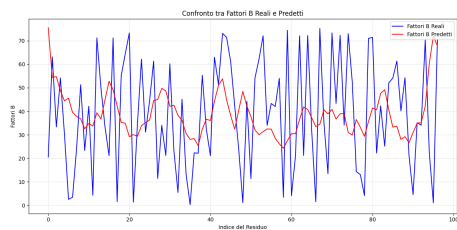


Figure 12: B factors

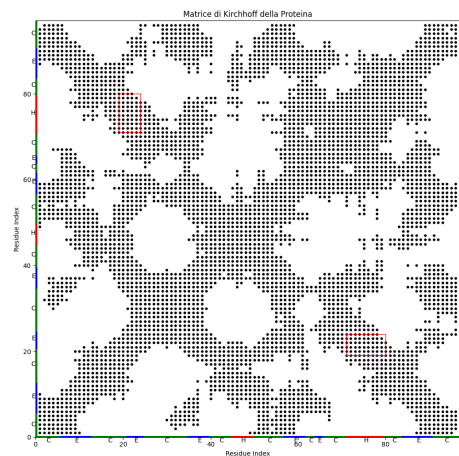


Figure 13: Kirchhoff

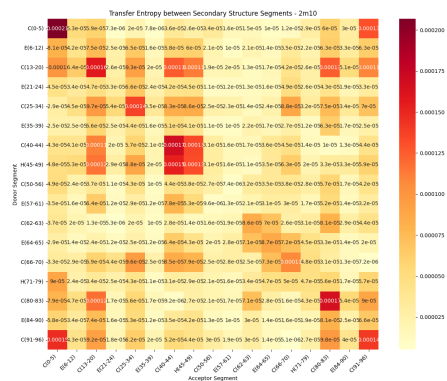


Figure 14: Transfer struttura Secondaria

8 3LNX

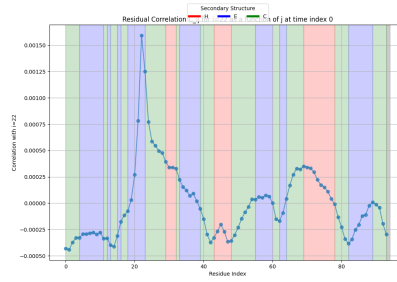


Figure 15: Correlazione

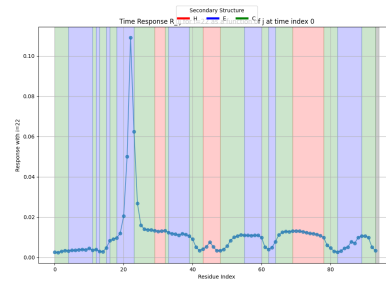


Figure 16: Risposta

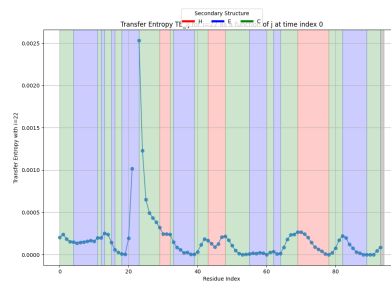


Figure 17: Transfer Entropy

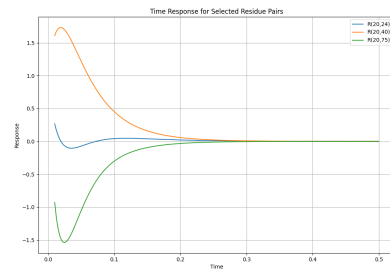


Figure 18: Multiple time response

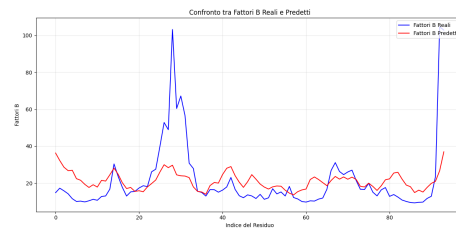


Figure 19: B factors

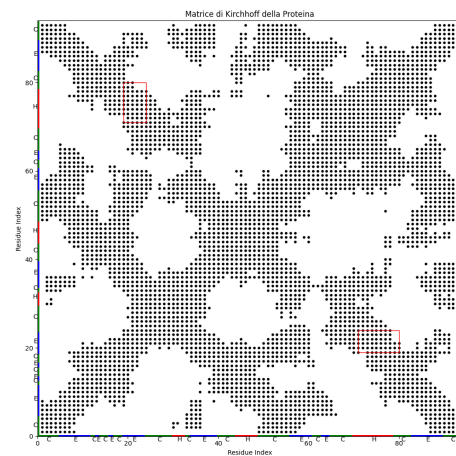


Figure 20: Kirchhoff

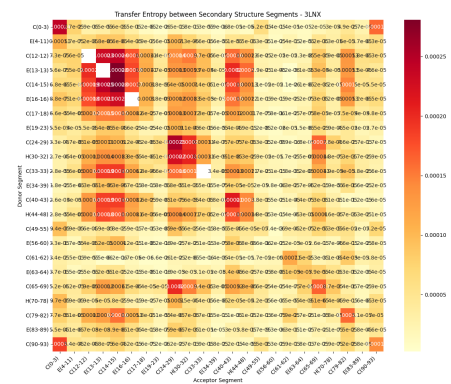


Figure 21: Secondaria

9 3LNY

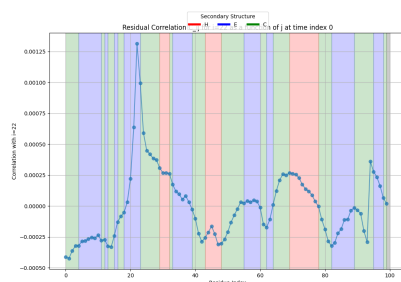


Figure 22: Correlazione

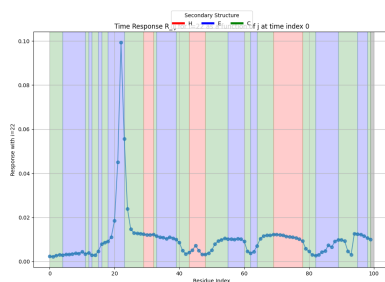


Figure 23: Risposta

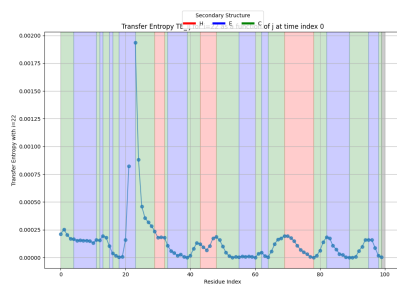


Figure 24: Transfer Entropy

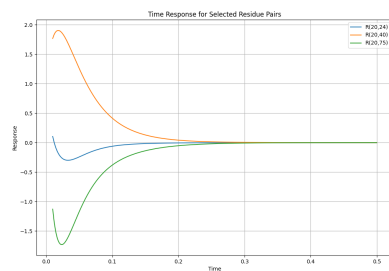


Figure 25: Multiple time response

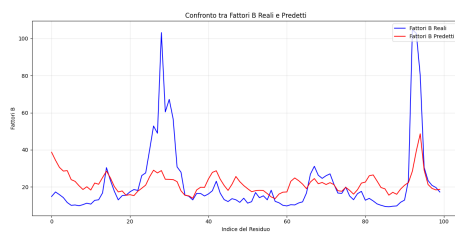


Figure 26: B factors

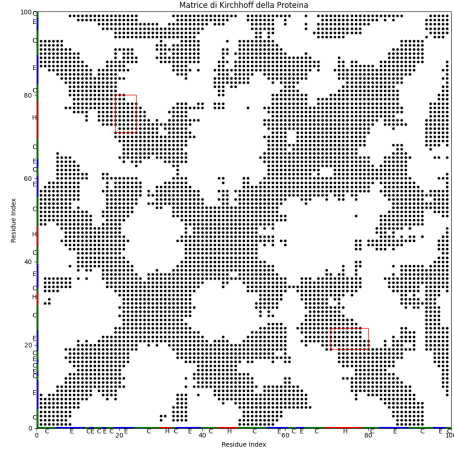


Figure 27: Kirchhoff



Figure 28: Seocndaria

10 Dinamica

$$\gamma \dot{x}_i = -g \sum_j K_{ij} x_j + \epsilon(t)(r_{21} - r_{76})\delta_{i,21} - \epsilon(t)(r_{21} - r_{76})\delta_{i,76} + \sqrt{2\gamma k_B T} \xi_i(t) \quad (15)$$

Ora posso simulare il moto Time dependent di ogni atomo e vedere come si propagano le vibrazioni. Gli autovalori sono smere le frequeze naturali del sistema.

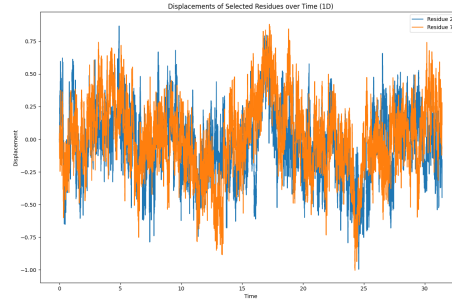


Figure 29: Seocndaria

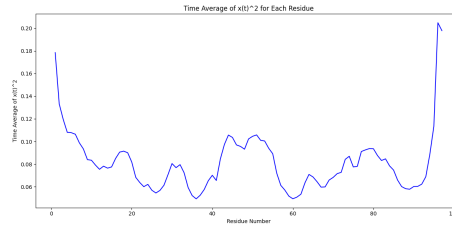


Figure 30: Seocndaria

11 Gradiente di temperature

$$\gamma_i \dot{x}_i = -g \sum_j K_{ij} x_j + \sqrt{2\gamma_i k_B T_i} \xi_i(t) \quad (16)$$

Gamma e T sono diventati vettori. Se la risolvi ottieni:

$$\sum_u \exp \left(\sum_j K_{ij} u_j \right) \cdot \beta \cdot \beta^\top \cdot \exp \left(\sum_s K_{is} u_s \right) \quad (17)$$

Ora hai diversi modi di scegliere i valori di T:

12 Troncamento Tmeperatura

se sono sotto 5 legami allora ho temperatura bassa. Se sono sopra allora ho temperatura piu' alta. Posso prendere banalmente 2 valori 0,1 .

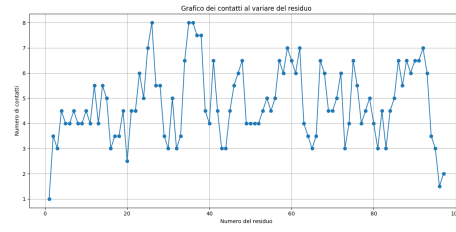


Figure 31: Temperatura Troncamento

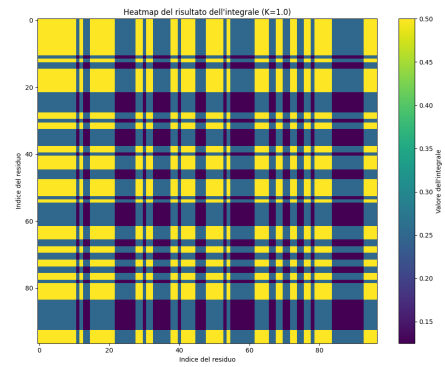


Figure 32: Temperatura Troncamento

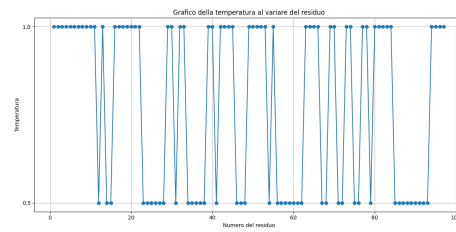


Figure 33: Temperatura Troncamento

13 Temperatura radiale

$$T(r)=T_0 + (Tb - T0)/R * r$$

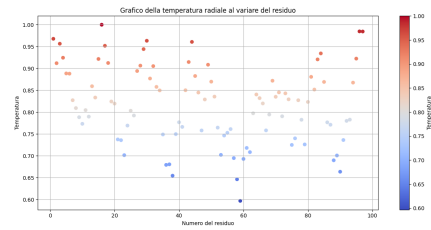


Figure 34: Temperatura Radiale

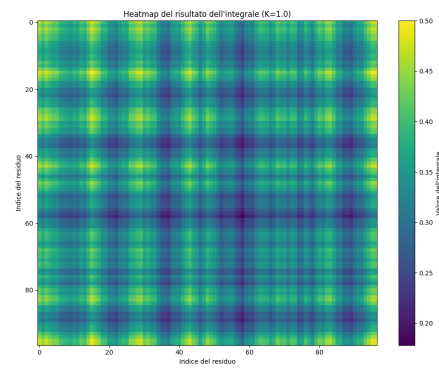


Figure 35: Correlazione Radiale