

## **Abstract**

Proteins are known to vibrate around their minimum energy structure. Hence these vibrations can be suitably modeled using harmonic oscillators. This framework uses the canonical ensemble to represent the protein around its equilibrium. The methodology is also called *Gaussian models* and is a topological model since most of the atomic details are neglected and importance is given only to the structure. This presentation will consist of a survey of recent developments in Gaussian models, discussing their predictability, verification and drawbacks. In the later half, a new model will be discussed which will try to rectify the drawbacks of the previous ones.

# Vibrations in proteins with prosthetic groups

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# Outline of Topics

Introduction

Gaussian models

Verification

The model description

Work done at SISSA

Results

# Vibrations in proteins

## ► Evidence

# Vibrations in proteins

- ▶ Evidence
- ▶ Importance

# Vibrations in proteins

- ▶ Evidence
- ▶ Importance
- ▶ Scope of the study

## Gaussian approach

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  - Solvent effects

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- ▶ Analysis
- ▶ Results

## Results, cont.

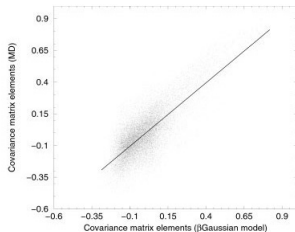


Figure: Comparison of the elements of the covariance matrix

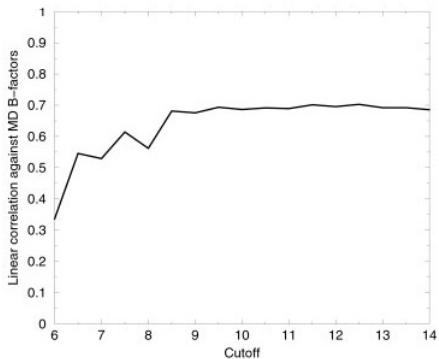


Figure: Optimum choice of cutoff

# Proteins with prosthetic groups

- ▶ Importance of the prosthetic group

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- ▶ System under consideration : Cytochrome C
- ▶ Drawbacks of the model



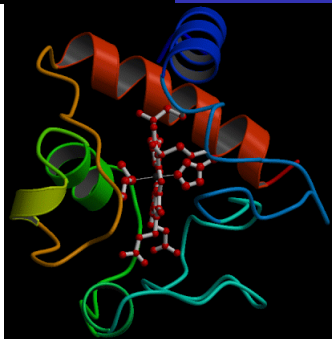


Figure: The 3-D structure of Cytochrome C

# Insights from allosteric mechanisms

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- ▶ Effective hamiltonian construction for Boltzmann distribution with quadratic hamiltonian
  - $\mathcal{H} = \mathbf{H}_1 - \mathbf{G}\mathbf{H}_2^{-1}\mathbf{G}^\dagger$

## Cutoff of 3.7 angstrom

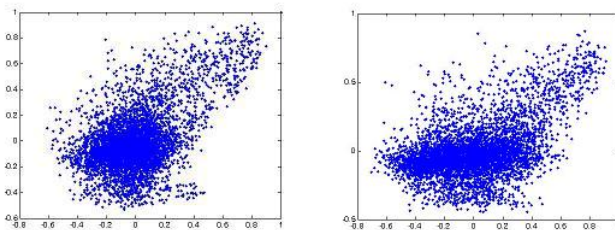


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## Cutoff of 3.8 Angstroms

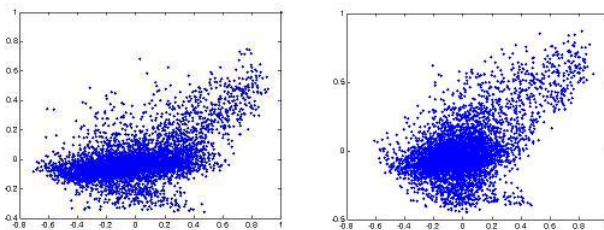


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## Cutoff of 4 Angstroms

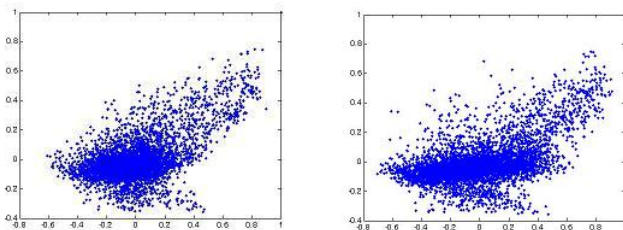


Figure: Comparison of the elements of the covariance matrix

## The two MD simulations

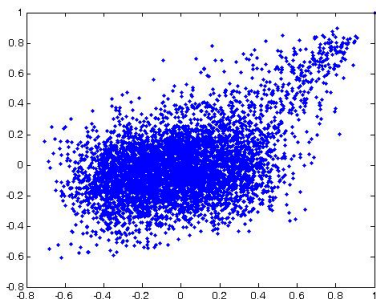


Figure: Comparison of the elements of the covariance matrix

Now this is not the end. It is not even the beginning of the end.  
But it is, perhaps, the end of the beginning.  
-Winston Churchill