

# NMA of Volumetric Data

**Pablo Chacón, Ph.D.**

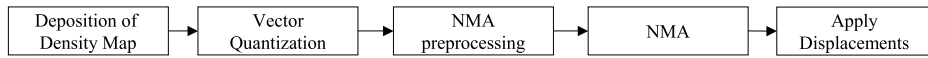
Department of Molecular Biology  
The Scripps Research Institute

10550 N. Torrey Pines Road, Mail TPC6

La Jolla, California, 92037

# RNA polymerase II (*E. coli*)

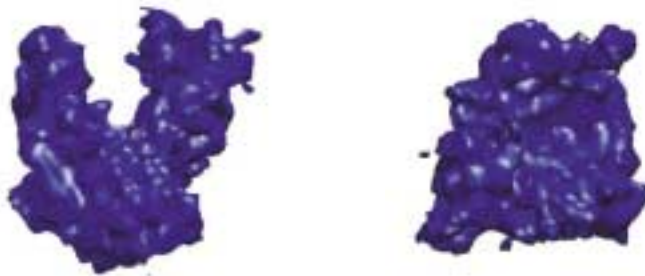
S. Darst et al.



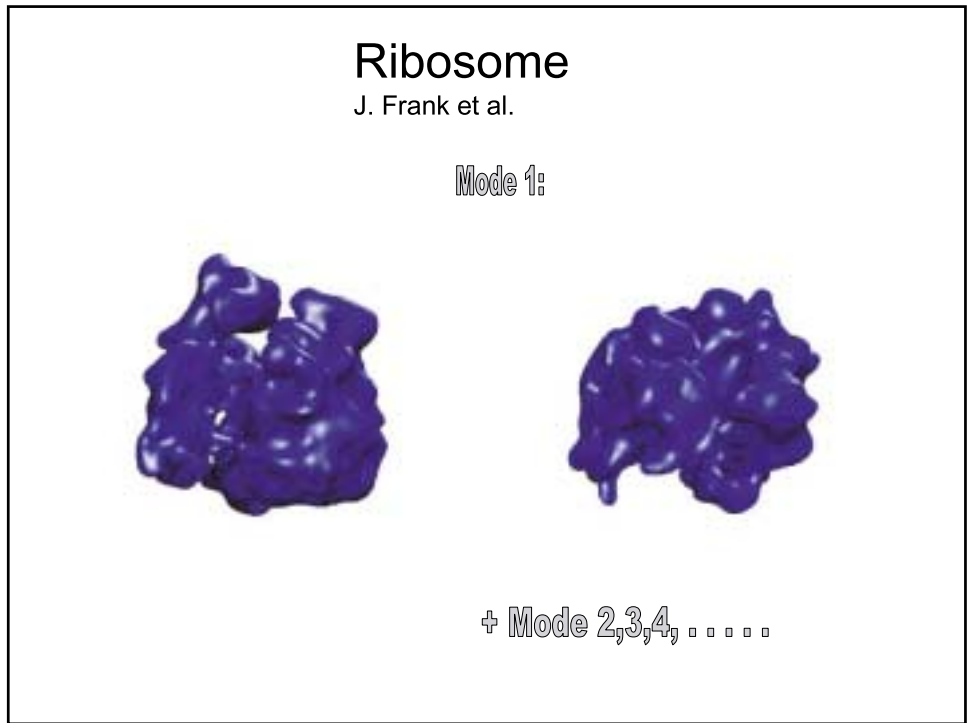
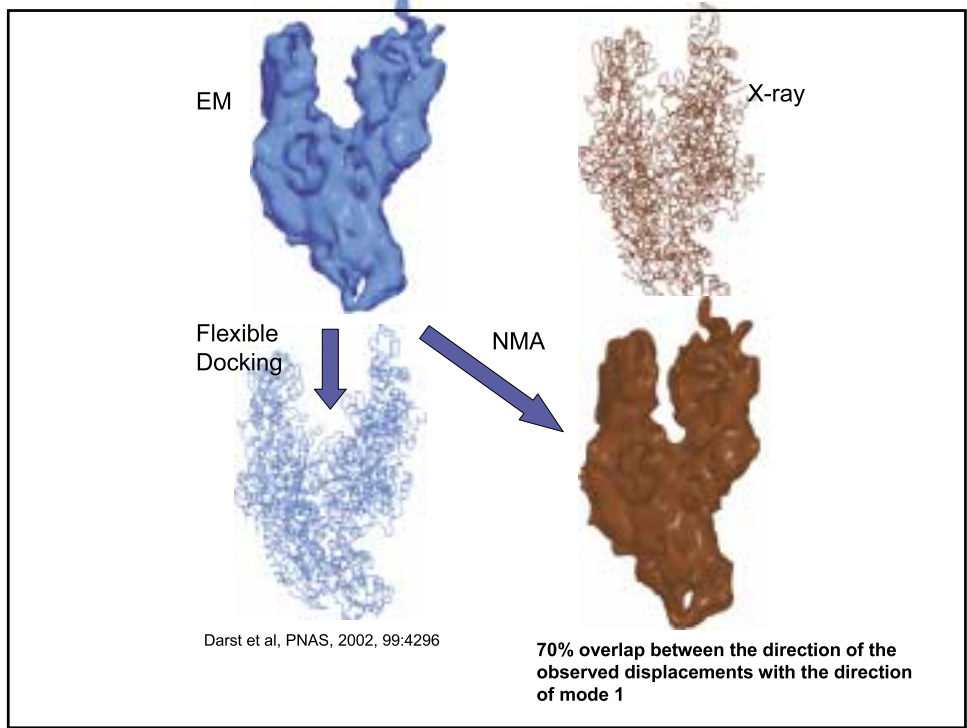
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Mode 1:



+ Mode 2,3,4, . . . . .



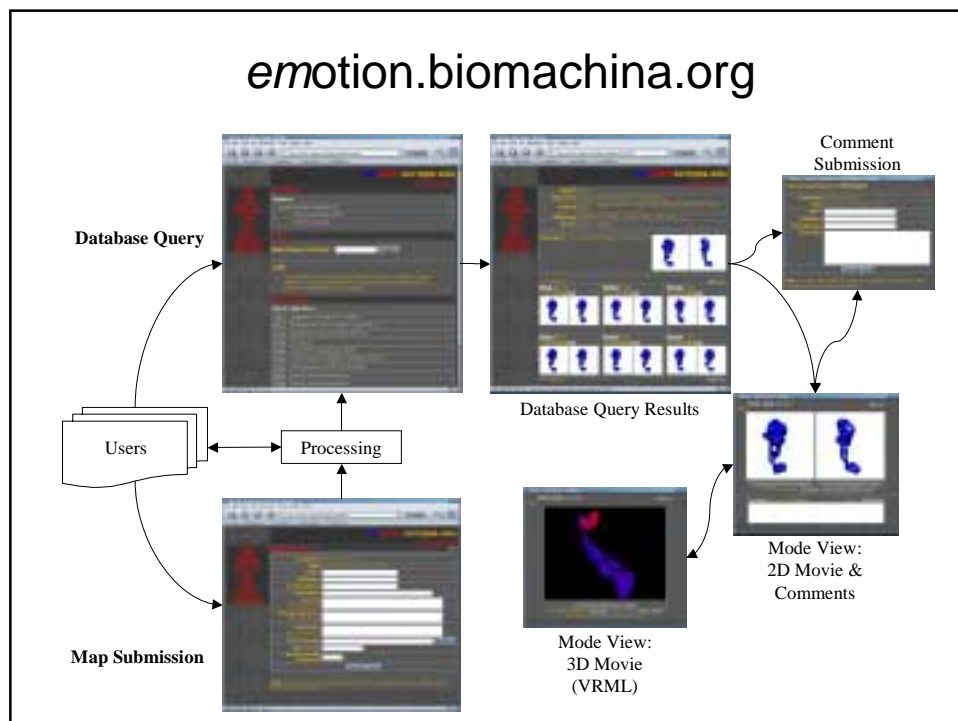
## What are the limitations?

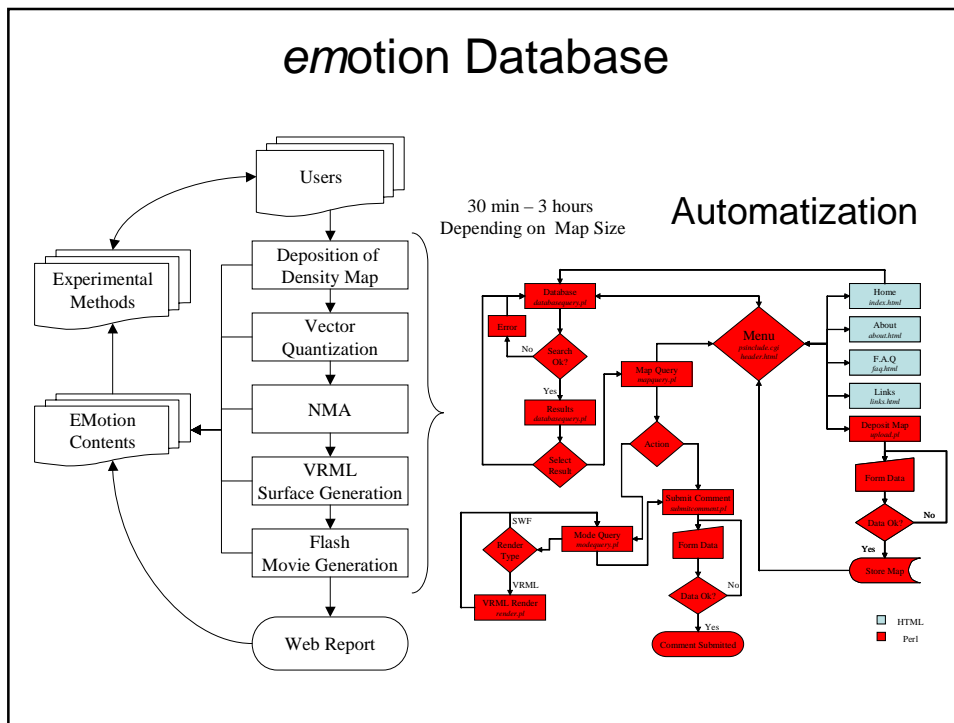
- We do not know *a priori* which is the relevant mode, but the first 12 low-frequency modes are probable candidates.
- The amplitude of the motion is unknown.

NMA requires additional standards for parameterization, i.e. a screening against complementary experimental data to select the relevant modes and amplitude.

Expert user input / evaluation

→ *emotion* movie database





## Applications

**Current - "as is":**

a tool for predicting functionally relevant motions  
 New URL: [emotion.biomachina.org](http://emotion.biomachina.org)

**Future - with complementary structural data:**

a tool to reduce the conformational search space.

**Flexible Docking:** Normal modes can be used as refinement parameters with low-dimensional complexity (planned for Situs 2.2)

**Image processing:** Normal modes can be added as additional degrees of freedom to capture polymorphism in the averaging and classification of EM images (collaboration with EM software developers).

# Acknowledgements

## PEOPLE:



Willy Wriggers { Essam Metwally (*emotion*)  
Julio Kovacs

C. Brooks III      Florence Tama

## FUNDING:

National Institutes of Health (R01 GM62968 and P41 RR 12255)

LJIS Interdisciplinary Training Program / Burroughs Wellcome Fund