



THE UNIVERSITY *of* TEXAS

HEALTH SCIENCE CENTER AT HOUSTON

SCHOOL *of* HEALTH INFORMATION SCIENCES

Term Paper Topics

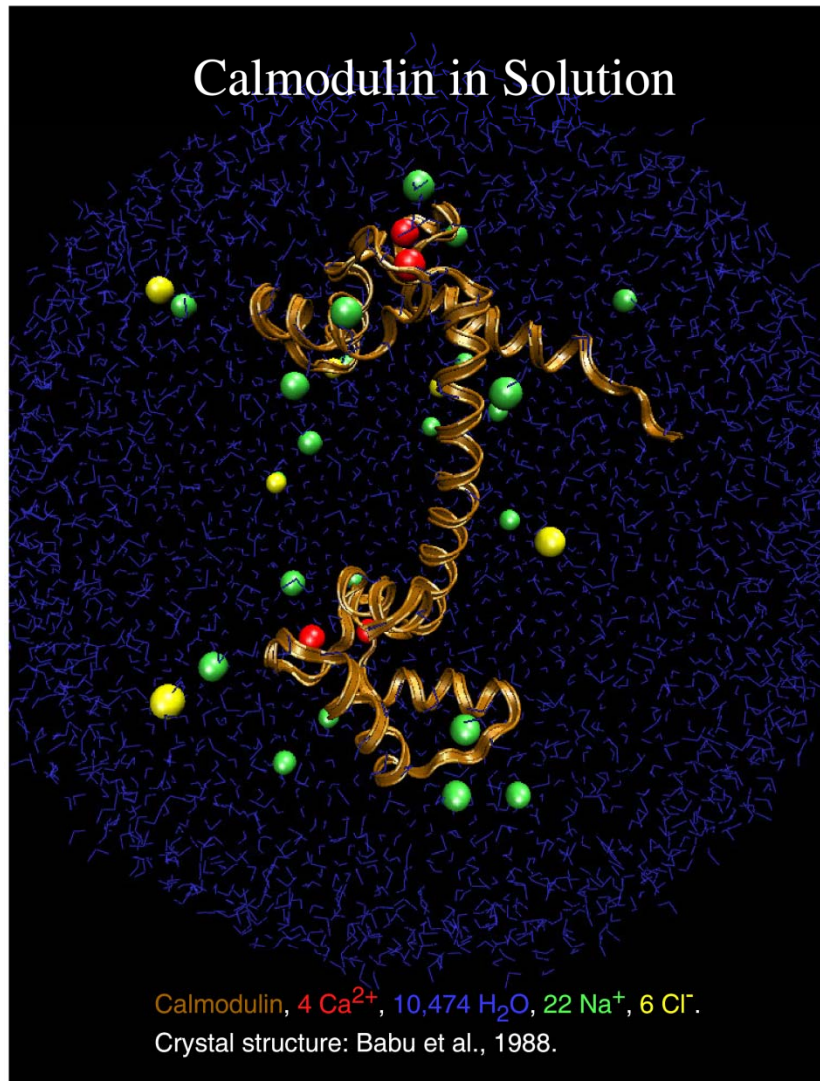
For students of HI 6327 “Biomolecular Modeling”

Willy Wriggers, Ph.D.

School of Health Information Sciences

<http://biomachina.org/courses/modeling/10.html>

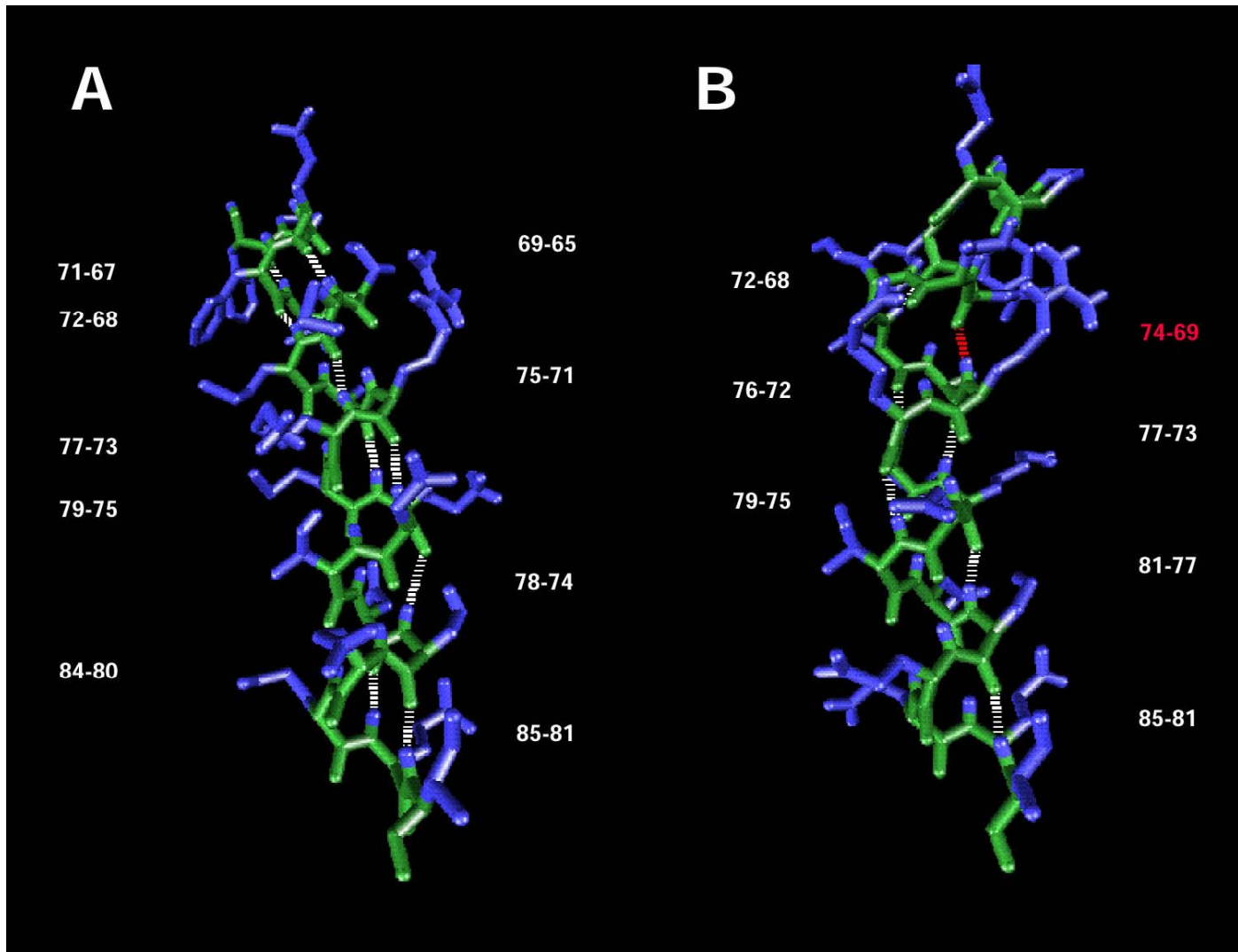
1. Calmodulin's Central Helix



central helix (res. 68-92) is highly flexible and “melts”

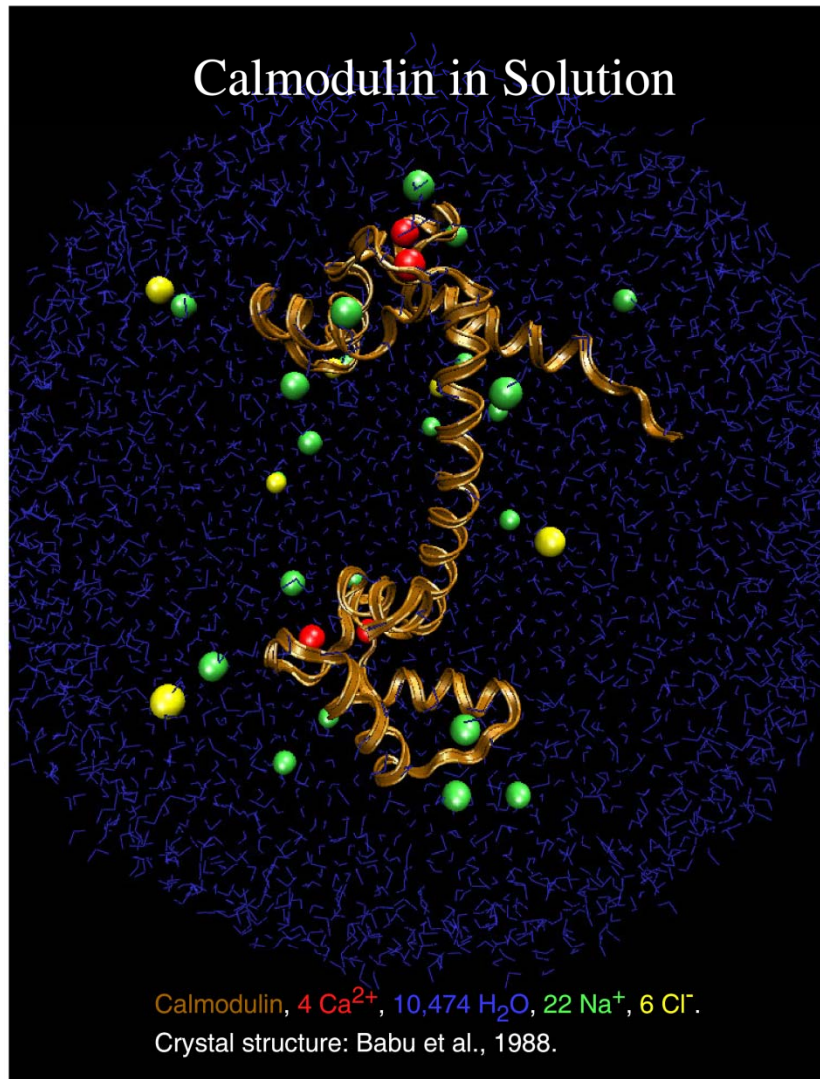
see: van der Spoel et al., Protein Science (1996)5:2044-53.

- extract helix from file provided
- solvate(6Å)
- heatup + MD (~1ns)
- differences between CHARMM19 and CHARMM22?
- different runs (seed of random number generator)



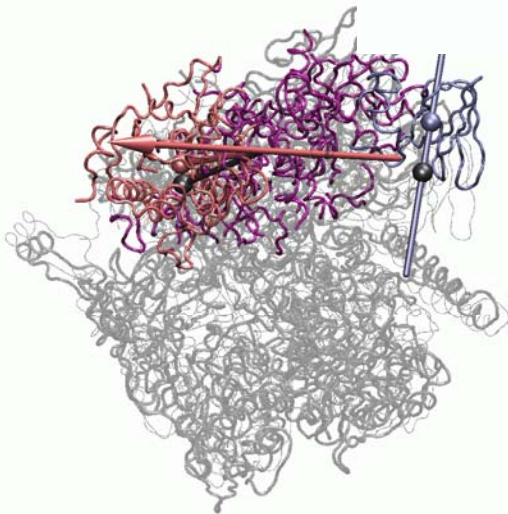
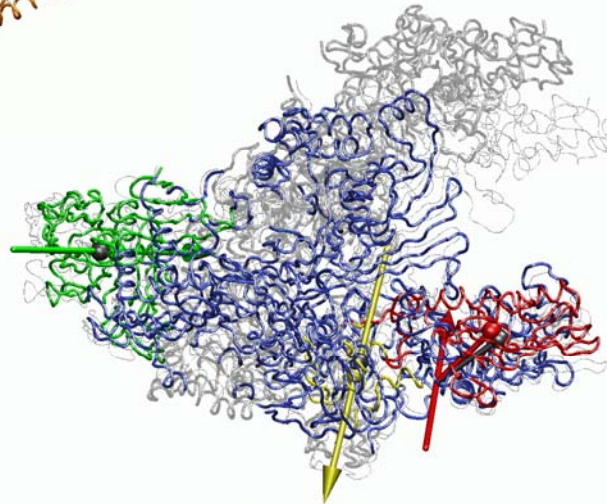
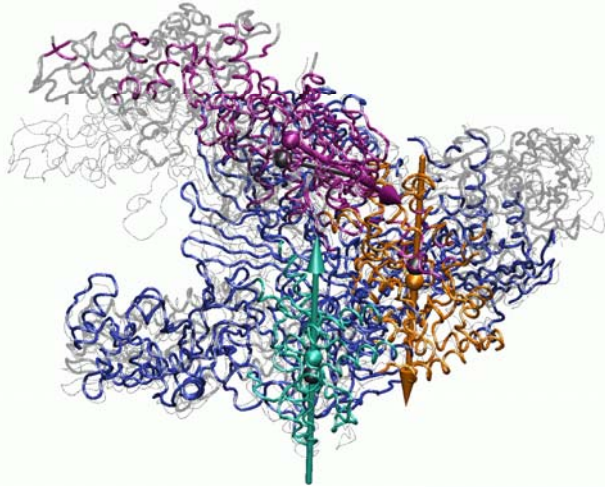
- explore hydrogen bonding patterns with VMD

2. Normal Mode Analysis



- extract protein only from file provided
- perform NMA using MMTK (<http://dirac.cnrs-orleans.fr/MMTK/>)
- visualize first 10 (non-trivial) modes, i.e. mode 7-16, with MMTK *vector fields* and compare qualitatively with motions published in http://www.biomachina.org/publications_web/WRIG98B.pdf

3. Hingefind



Compare both VMD and X-PLOR implementations of *hingefind* script using various levels of tolerance and various options, on the two provided RNA polymerase files

Flexing paper
(two conformations):
http://www.biomachina.org/publications_web/DARS02.pdf

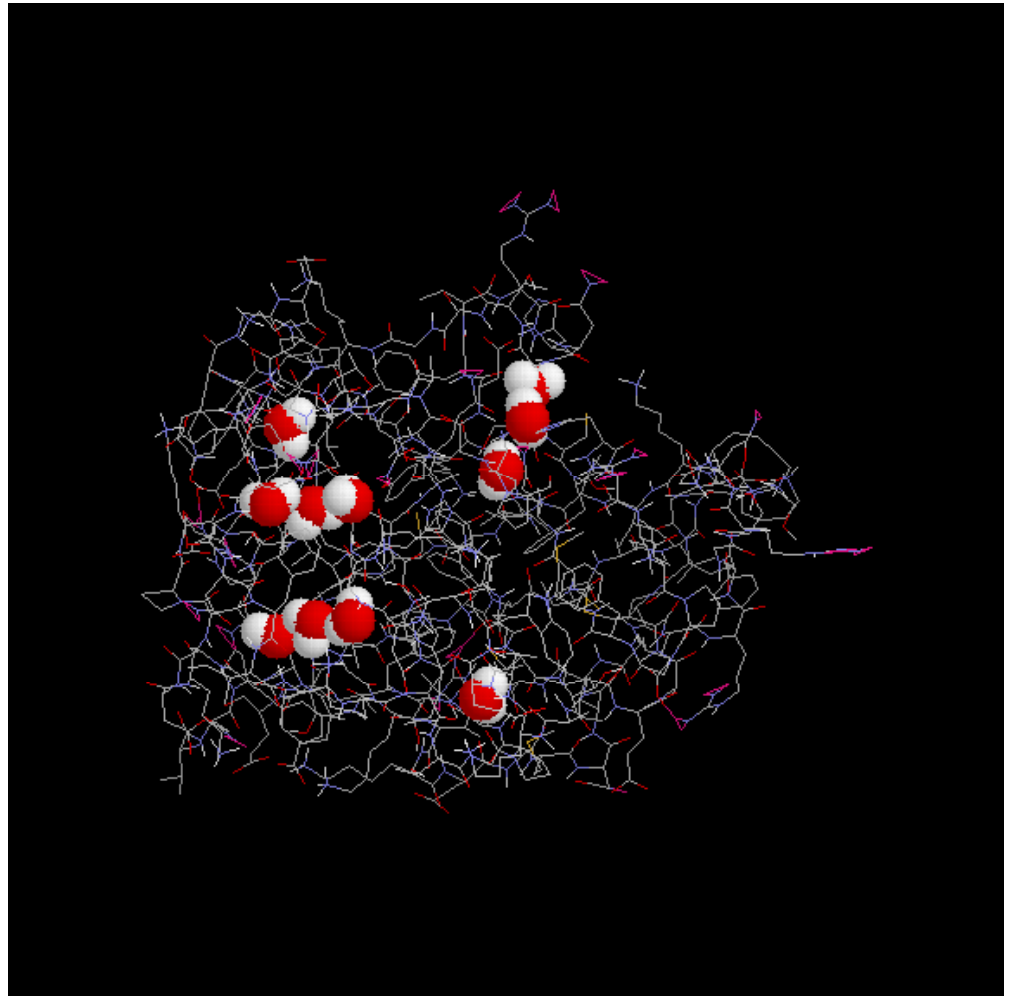
4. Dowser

To prevent collapse of any cavities, we need to fill them with water molecules

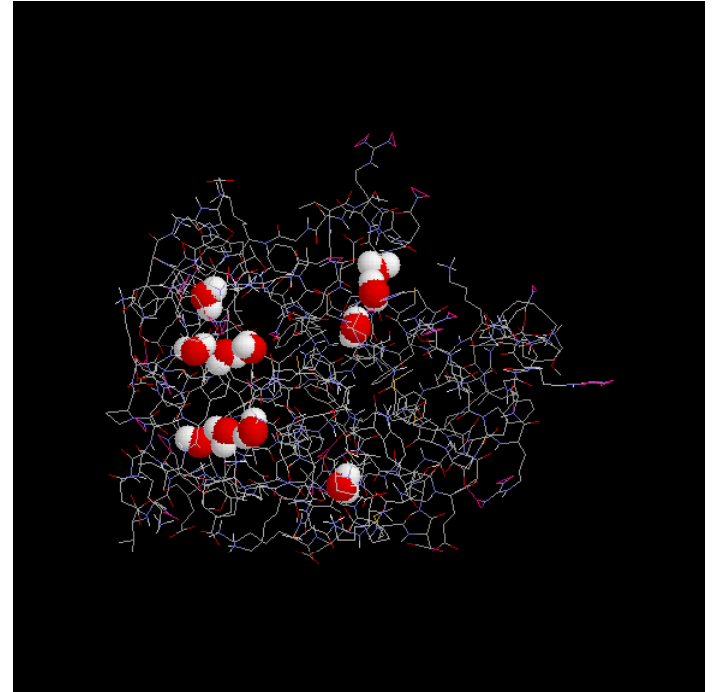
DOWSER program (Jan Hermans, UNC Chapel Hill)

URL:

<http://hekto.med.unc.edu:8080/HERMANS/software/DOWSER/>



- pick protein of your choice from PDB
- must have at least 10 buried waters (Dowser)
- then use solvate.inp for surface water (6\AA)
- compare MD (heatup+100ps) results for empty and filled cavities. Plot radius of gyration as function of time (see X-PLOR manual)



5./ 6. Per Agreement

- Coarse-grained Normal Mode Analysis (Rhys)
- Flexible Docking Program (Mirabela)