Simulation of Molecular Machines

A Simbios Home Run (Sherm)

Examples

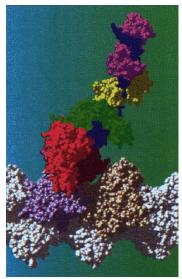
- Enzymatic action via conformational change
- RNA & protein folding, myosin mechanics, RNA transcriptase
- Membrane interaction, protein/RNA complexes
- Ultimately: electron transport chain, ribosome operation

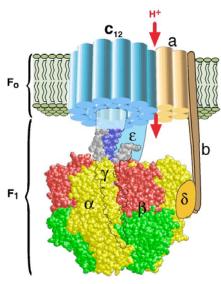
Characteristics

- Significant time scales
- Reveals previously unknown mechanistic details
- Correct prediction of experiments before they're done
- Must be useful to people who actually study molecules!

What will it take?

- Coarse grained but physically accurate models
- Best of classical & statistical mechanics, numerical methods
- Fast, high fidelity force fields (mixed continuum & discrete)
- Specialized applications & full exploitation of cheap hardware
- Timeline: significant results in 4 years, dramatic in 10
 - We are moving in this direction already





H. Wang and G. Oster (1998). Nature 396:279-282.