

# Simulation of Molecular Machines

## A Symbios 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

