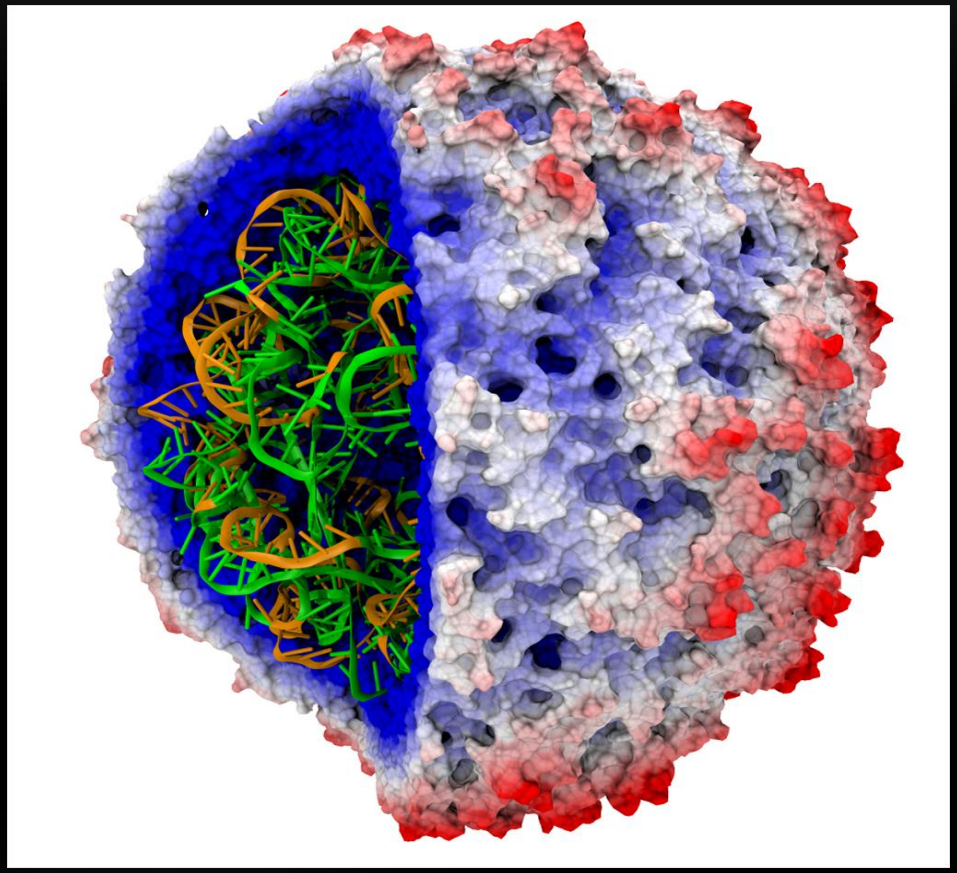
MOLECULAR DYNAMICS SIMULATION OF SELF-ASSEMBLY OF SPAN 80

SHANE LINDEMANN

- Mentor: Dr. Moldovan Mechanical Engineering Dept.
- Originally from Pahrump NV
- LSU
  - Sophomore
  - Physics

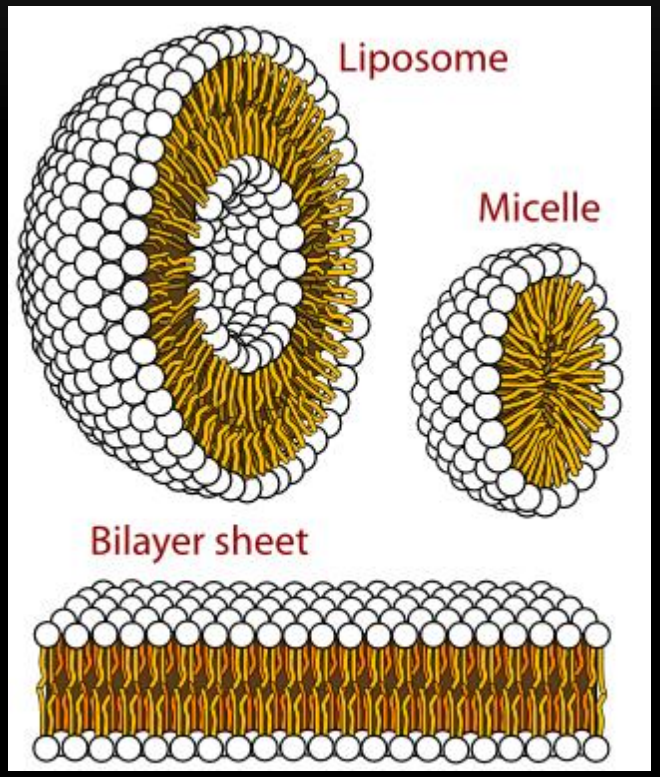
MOLECULAR DYNAMICS

- What is MD???
  - Atoms/molecules and their interactions/move-ment
  - What they do, how they get there
    - Trajectories
  - Uses computer simulations

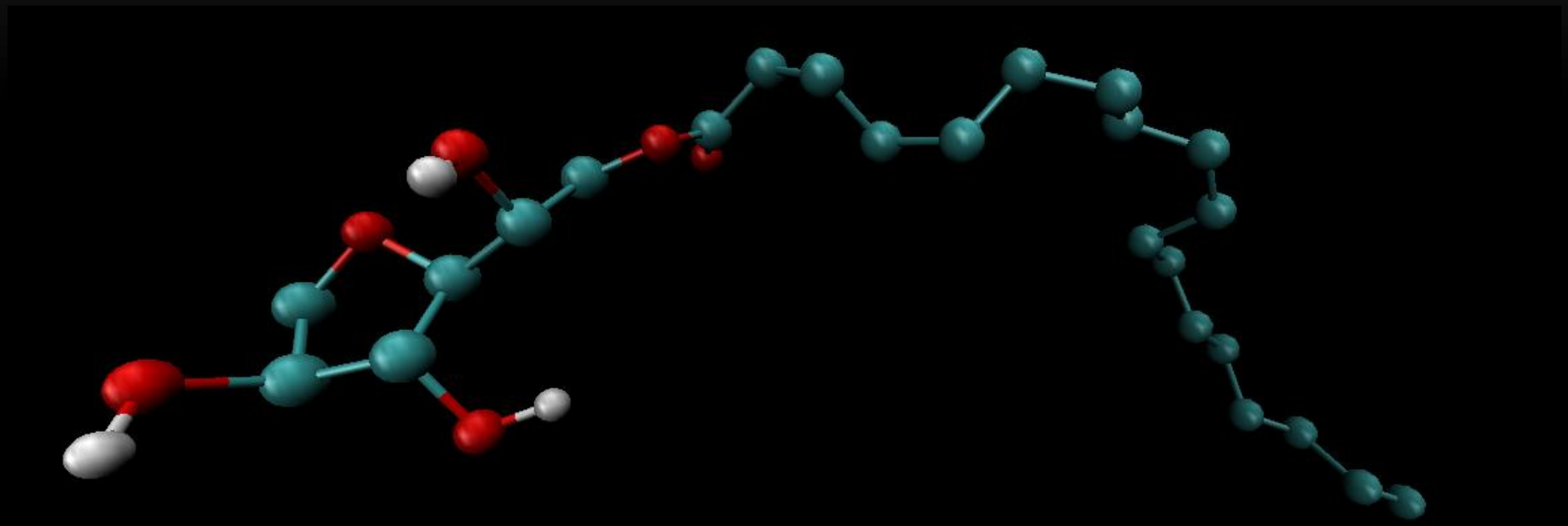


SPAN 80

- Surfactant
  - Micelle then vesicle
    - Examples of where this formation is found
    - Analyze/quantify MD of this process



SPAN 80 (33 ATOMS)

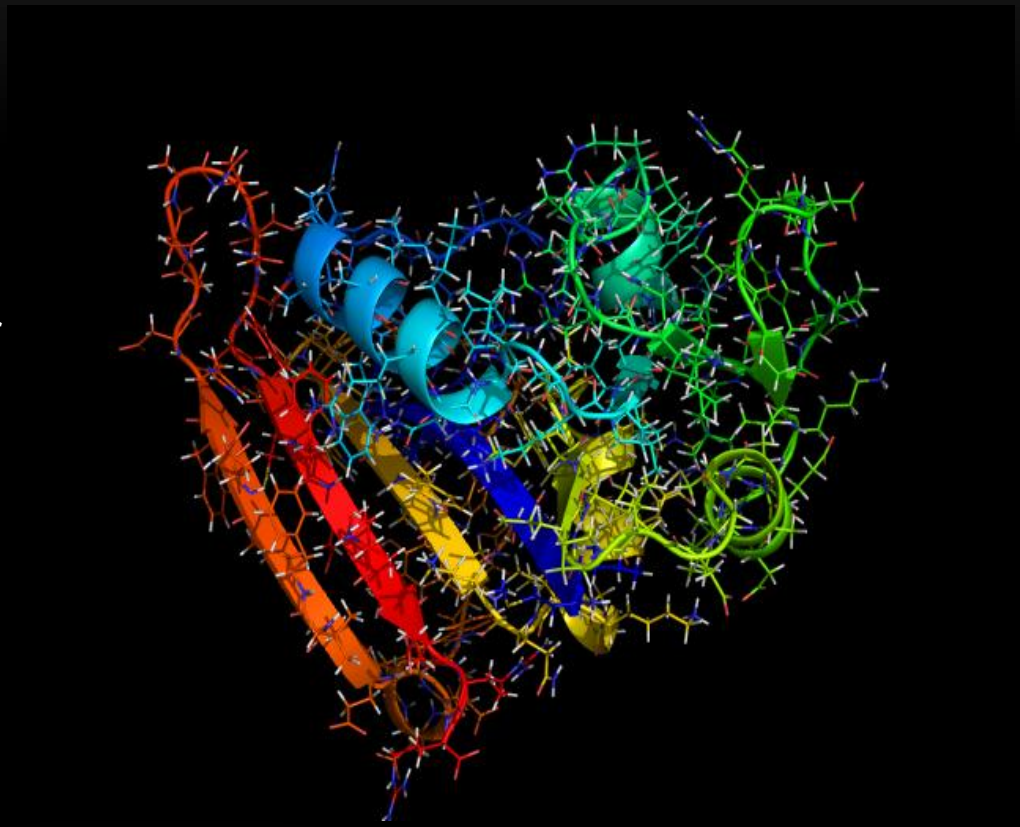


PROCEDURE

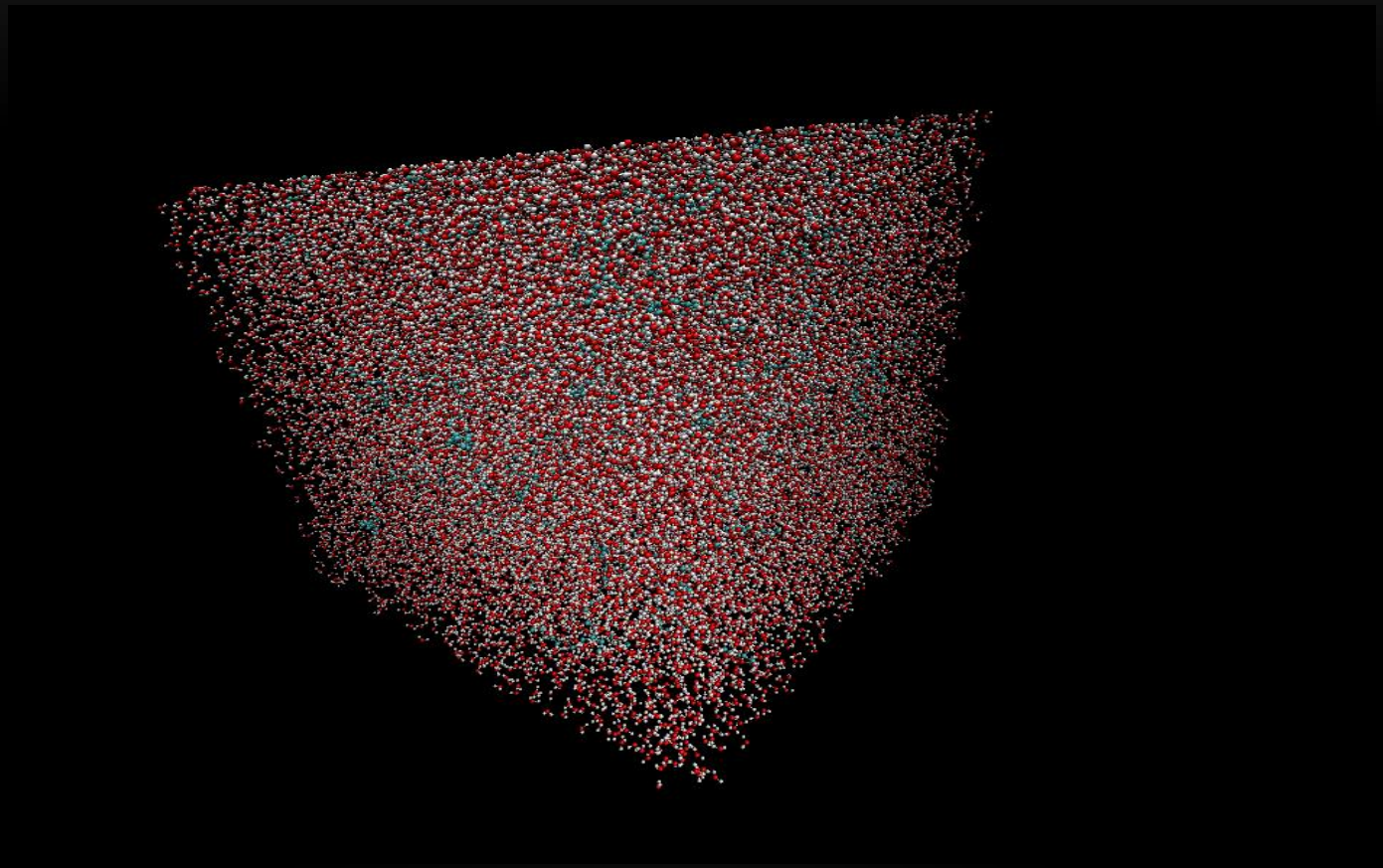
- Start with files for each molecule. (H_2O and Span 80)
- Create structure file
  - Packmol
- Run energy minimization
- Set up run script
- Submit job to super computer
  - Gromacs

GROMACS

- Does most of the simulation
  - Uses parallel processors (super computing)
  - Simulations are run based off Newtonian Equations for systems of hundreds to millions of particles



INITIAL STRUCTURE



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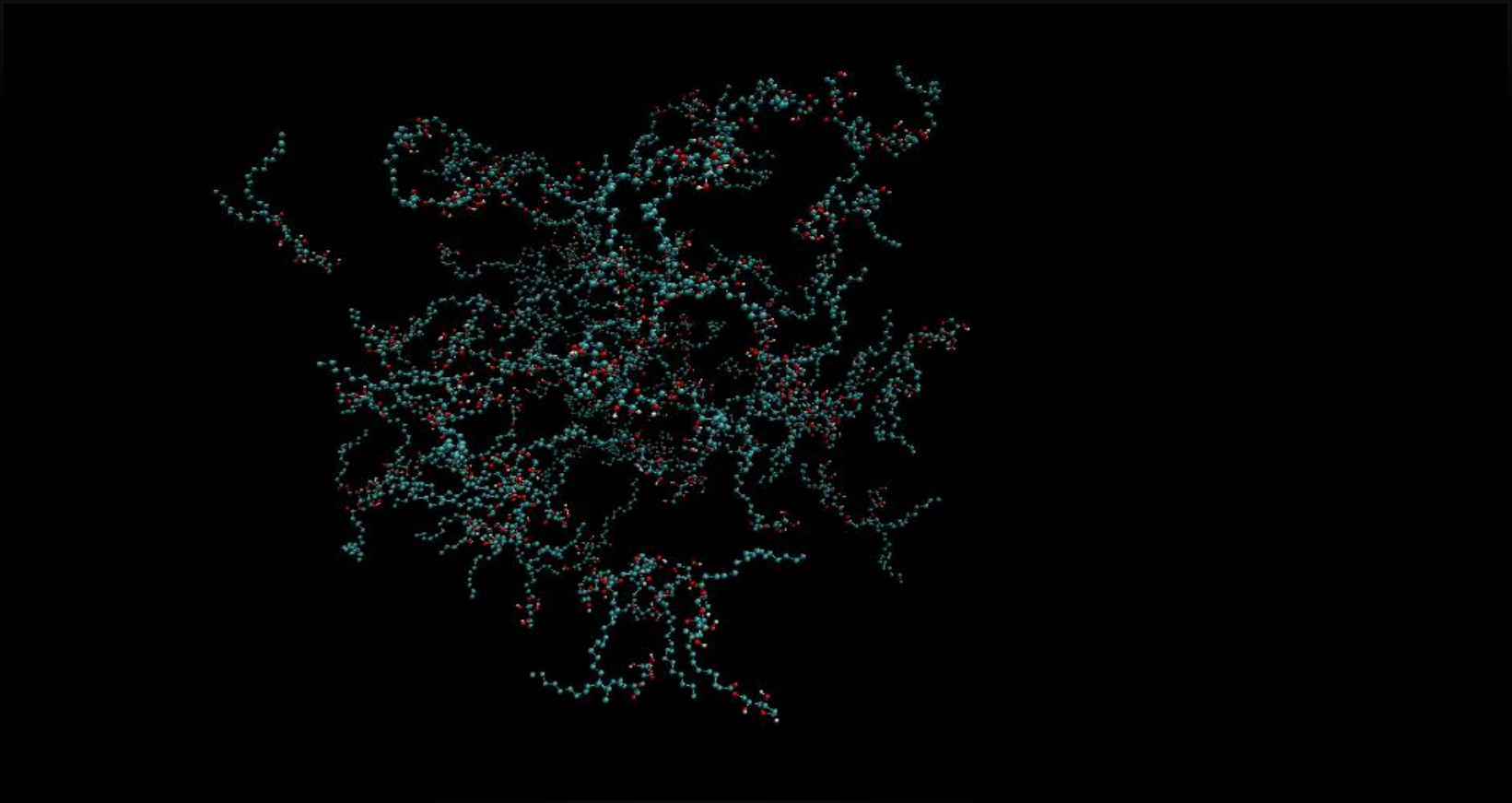
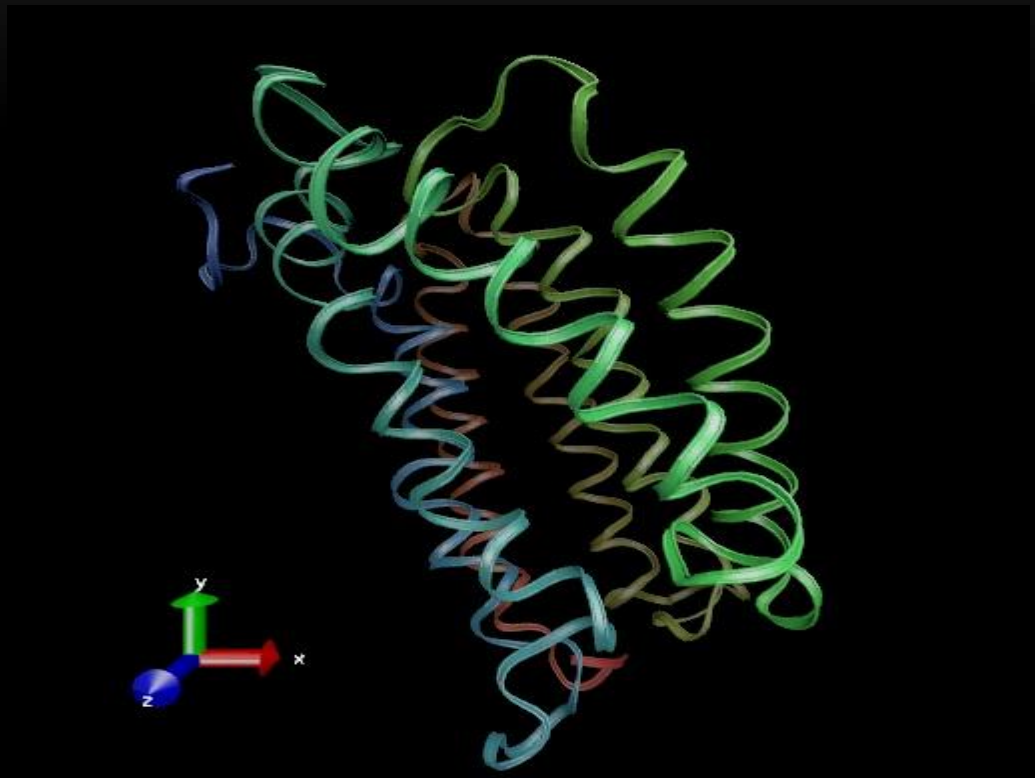


NOW 7/20/11

- Simulation is running on Super computer.
  - Max 3 days at a time
    - Hopefully 20 ns
  - Resubmitted for 3 more days
- When finished simulating
  - Visualize the results (VMD)
  - Quantify the clustering effect of Span 80
  - Hopefully see some nice vesicles

VMD

- Visual Molecular Dynamics
  - What it does
    - Visualizes



QUESTIONS???