Department of
PHYSICS *and*
ASTRONOMY

Molecular Dynamics Simulations of Collagen

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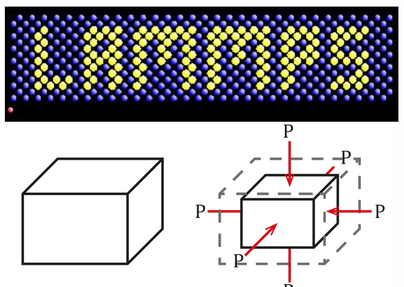
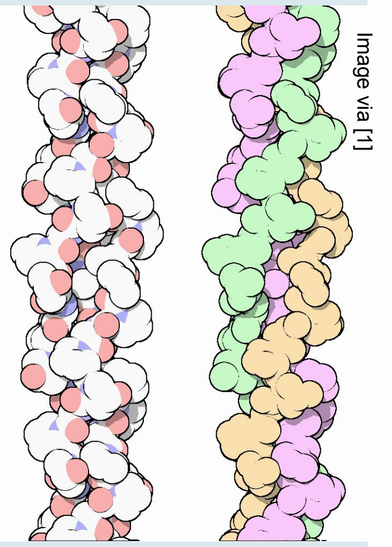
Introduction

Roughly 30-40% of the proteins in your body are collagen. Collagen provides structural and biochemical support to the extracellular matrix (ECM). Changes in the stiffness of the ECM can have effects on the structural integrity of the ECM, cell motility within the ECM, and cell diversification. In the lab we can measure the structural properties (bulk modulus, shear modulus) of collagen using Brillouin spectroscopy. Additionally, we can use molecular dynamics simulations to measure the same moduli. Here, molecular dynamics simulations performed using the LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) code are used with the goal of replicating and then aiding experimental results made using Brillouin spectroscopy in the lab. As both tissues and our simulation environment are largely made of water we expect a similar bulk modulus around 2 GPa and a shear modulus about an order of magnitude lower. This poster is largely based on the current progress of the simulation and future steps to be made towards the simulations improvement.



Bulk modulus:

$$K = -V\frac{dP}{dV}$$



Procedure

- Build data file
  - Includes locations, bonds, charge, etc...
  - Forcefields provided via CHARMM
- Write LAMMPS input script
  - Built from example script
  - Deforms simulation box and measures the resulting changes in force to calculate moduli
  - LAMMPS integrates Newton's equations of motion for a collection of interacting particles
- Run script on computing cluster
  - UNC's dogwood computing cluster allows for parallelization of simulation
- Interpret the results

Progress

Past problems and solutions:

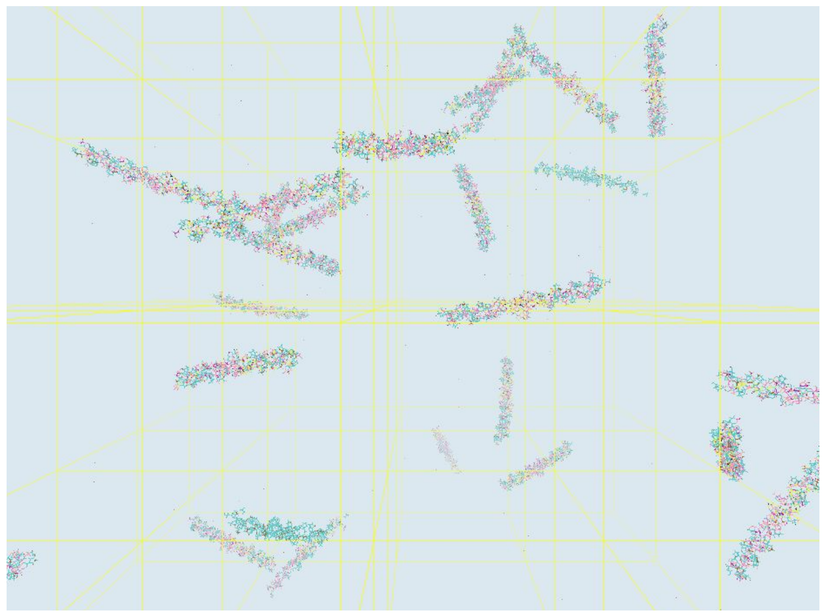
Problem: An overabundance of water molecules slows down the simulation time.
Solution: Nonstructural water was removed and treated as an implicit solvent.

Problem: The system was not charge neutral due to removing of atoms.
Solution: Ions are added to neutralize system.

Problem: Some bonds expand rapidly when the simulation step size is increased.
Solution: Implement the SHAKE algorithm to constrain bond lengths.

Current problems:

- Mismatched bond atoms in input file.
- Increasing the size of the simulation box leads to significant slow downs.

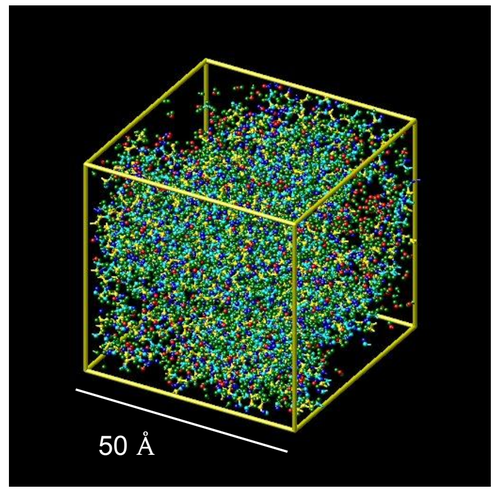


***Current Simulation Box*:**
Current simulation box filled with 28 collagen-like proteins. Grid markers occur every 125 Å.

Goals

Short Term:
- Update input files
- Increase simulation time step
- Fix parallelization issues

Long Term:
- Implement higher order structure of collagen
- Simulate enzyme via removal of bonds



***Former Simulation Box*:**
Formerly the simulation consisted of a single collagen-like protein surrounded by water. Each simulation box dimension is 50 Å.

Acknowledgements

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References

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