

## **Molecular Dynamic Simulations of Collagen**

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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.