Actin and Filamin Simulations Using the Metropolis Monte Carlo (MC) Algorithm

Terry Salava Jr

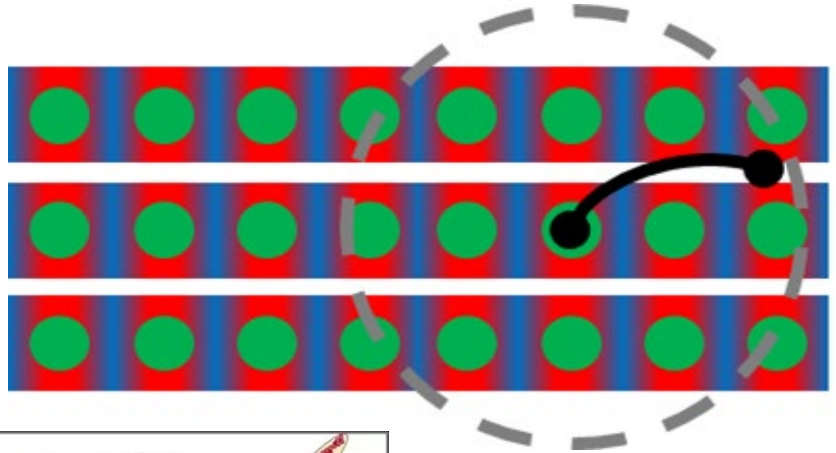
August 2nd 2019

Kamal Bhandari and Jeremy Schmit

F-Actin and Filamin

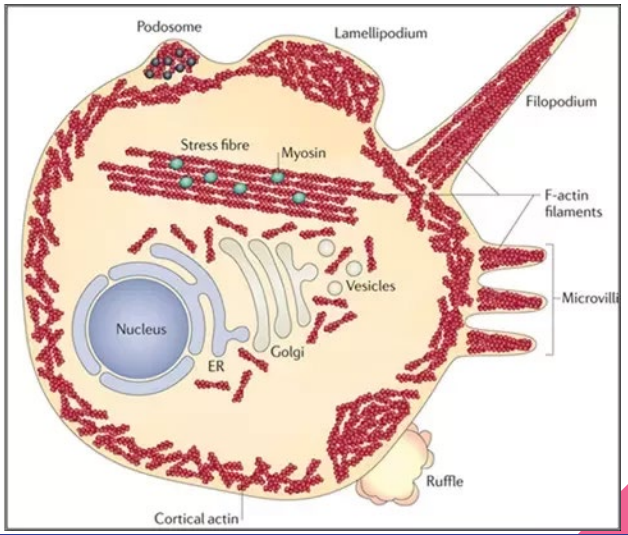
F-Actin found in the cytoskeleton

Long straight protein with many bonding sites



Filamin bonds with Actin

Only has 2 bonding sites



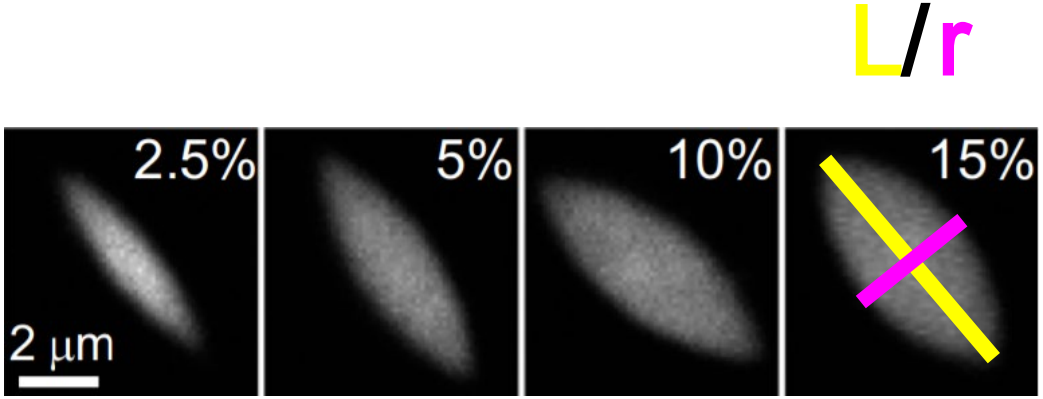
https://www.quora.com/Are-microfilaments-of-cytoskeleton-attached-to-proteins-on-outer-surface-of-cell-membrane

Actin and Filamin Mixture

When actin and filamin are mixed they form a droplet

The aspect ratio of the droplet changes with concentration

Are the macroscopic properties related to microscopic properties



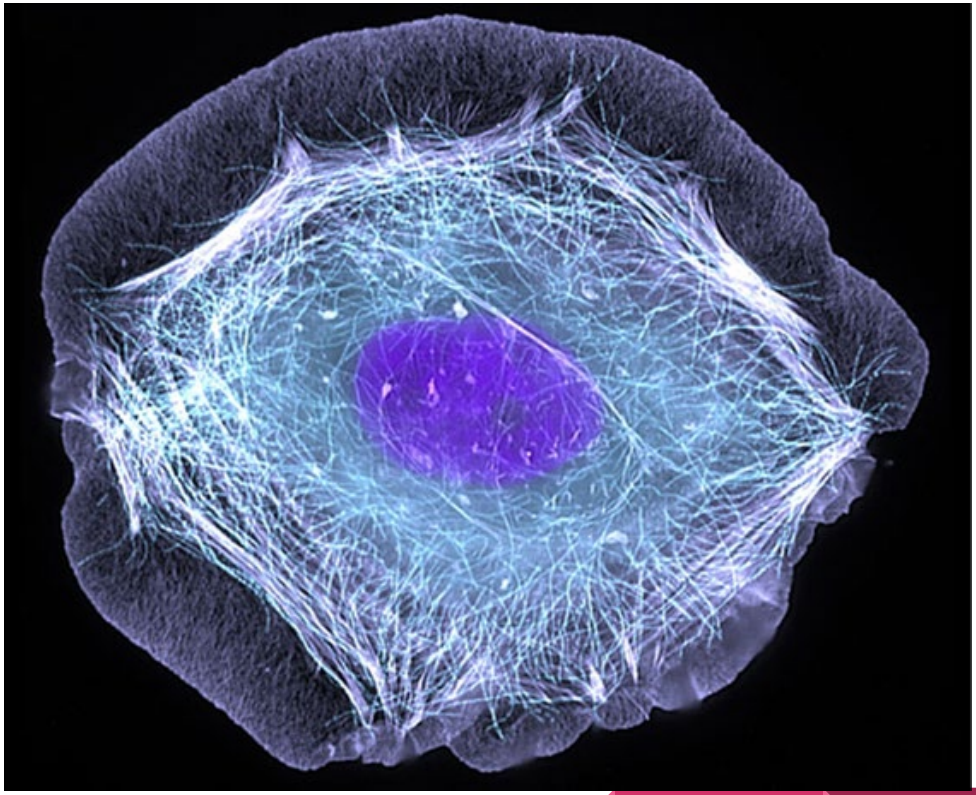
"Liquid Behavior of cross-linked actin bundles" Weirich et al.

Goal

Use Monte Carlo Simulation to generate random states

Measure the aspect ratio (L/r) of the droplets and average them

Understand the structure of a protein droplet, how it connects to macroscopic measurements.



https://www.sciencenewsforstudents.org/article/nanostraws-safely-sneak-peek-inside-cells

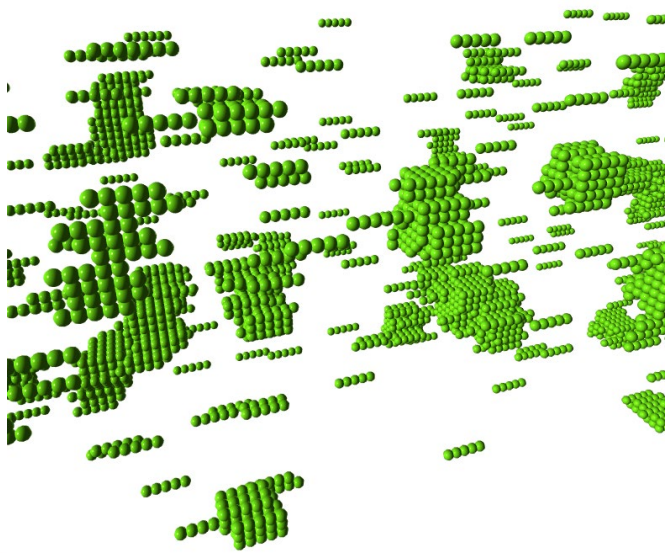
My Simulations

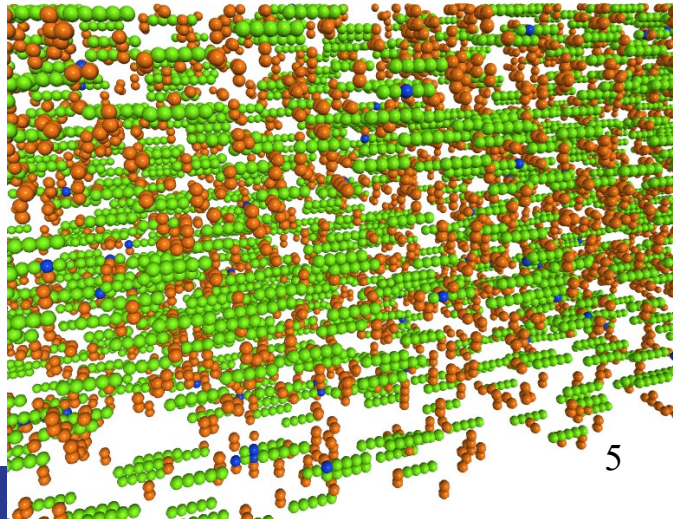
Single protein simulation (F-actin only)

- Shorter run time
- Bonds with adjacent proteins
- Filamin simulated implicitly

Two protein simulation (F-actin and Filamin)

- Longer run time
- Bonds only if both proteins occupy the same space
- Filamin simulated explicitly





The Metropolis Monte Carlo Algorithm

1)Choose an initial state

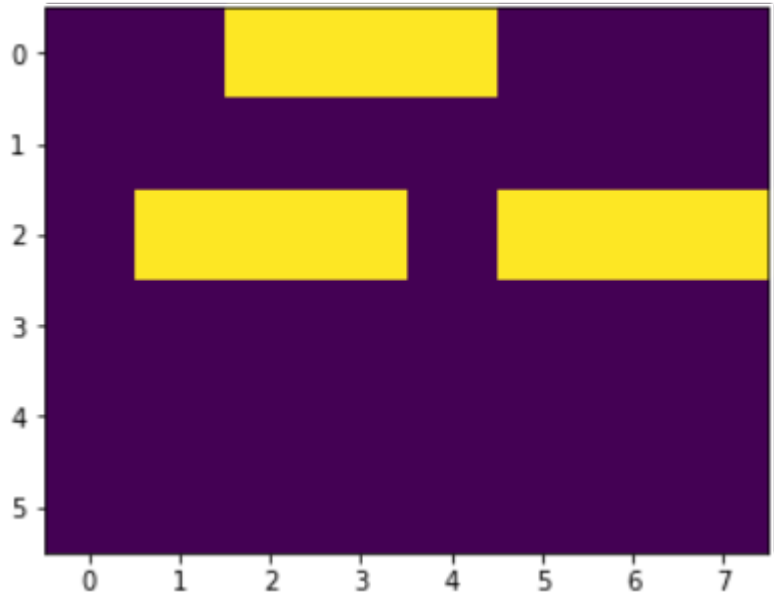
2)Choose a random site i

3)Calculate the ΔE if site i were to change

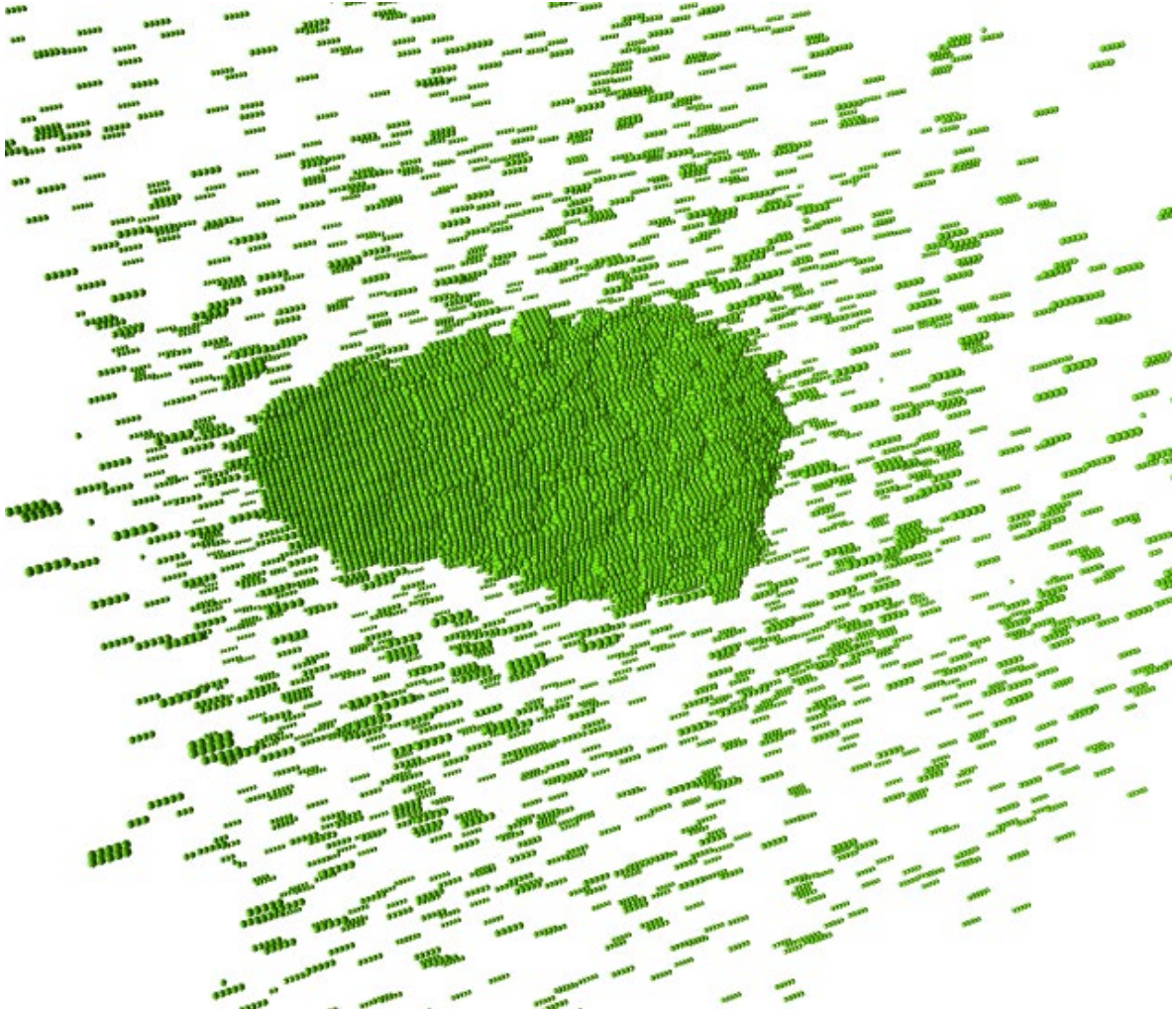
4)Generate a random number $0 \leq r \leq 1$

5)If $r < e^{-\Delta E}$ accept the new position

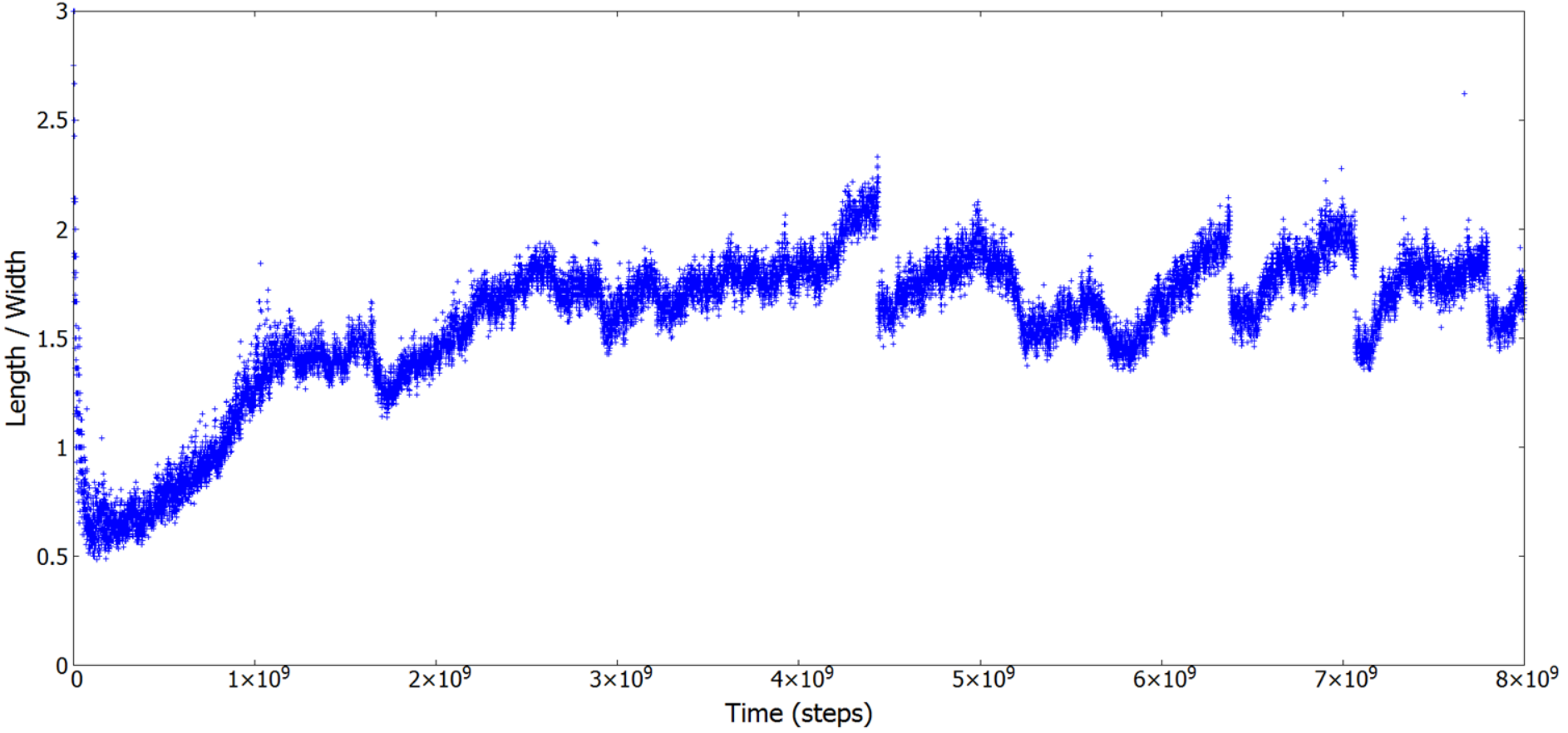
6)Repeat from step 2

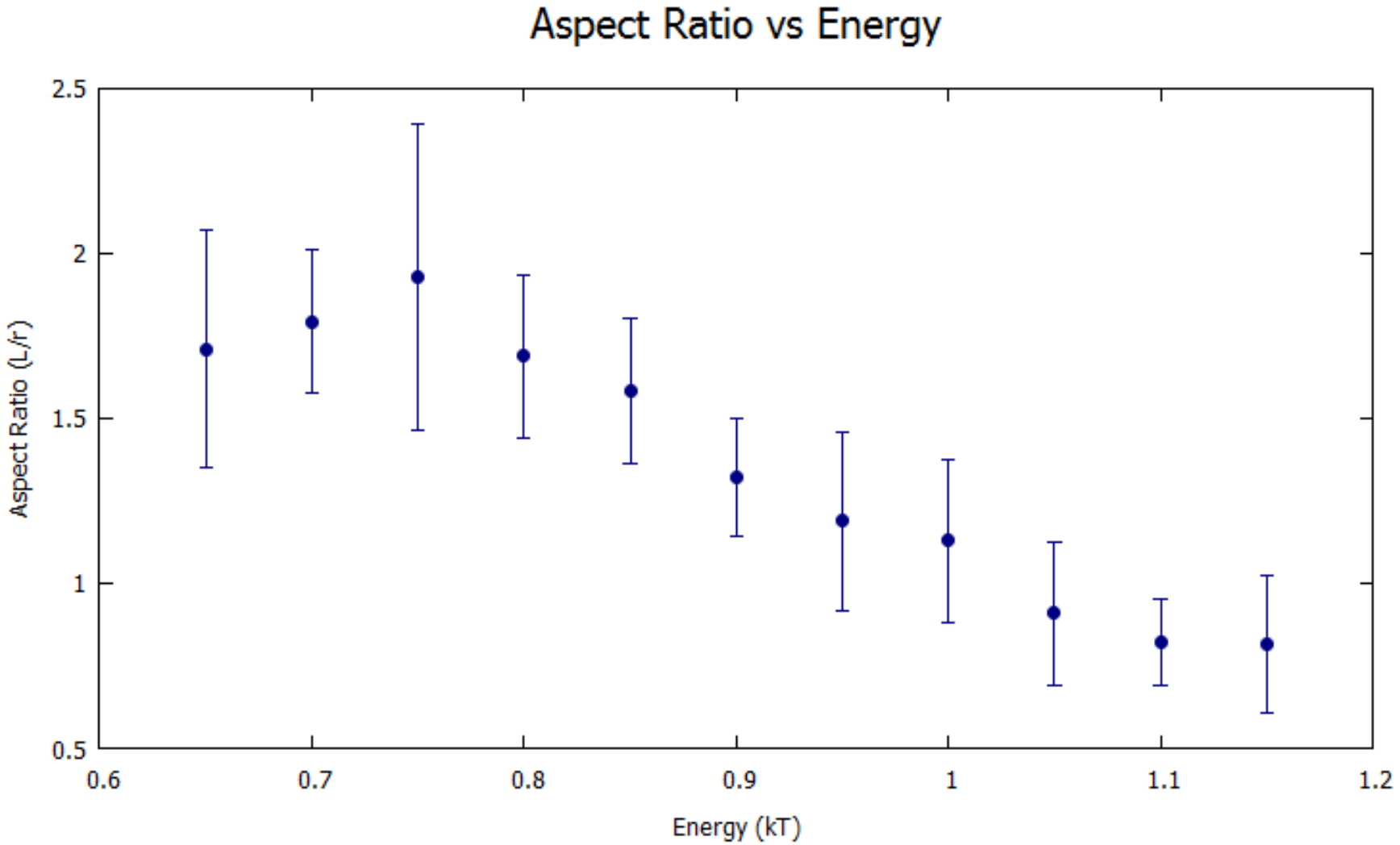


Method from "A Guide to Monte Carlo Simulations in Statistical Physics"

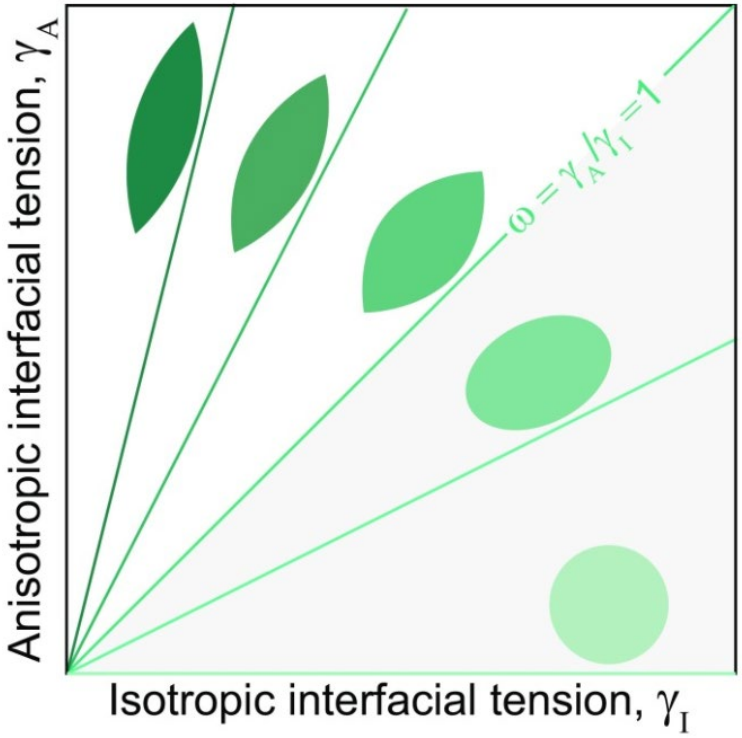


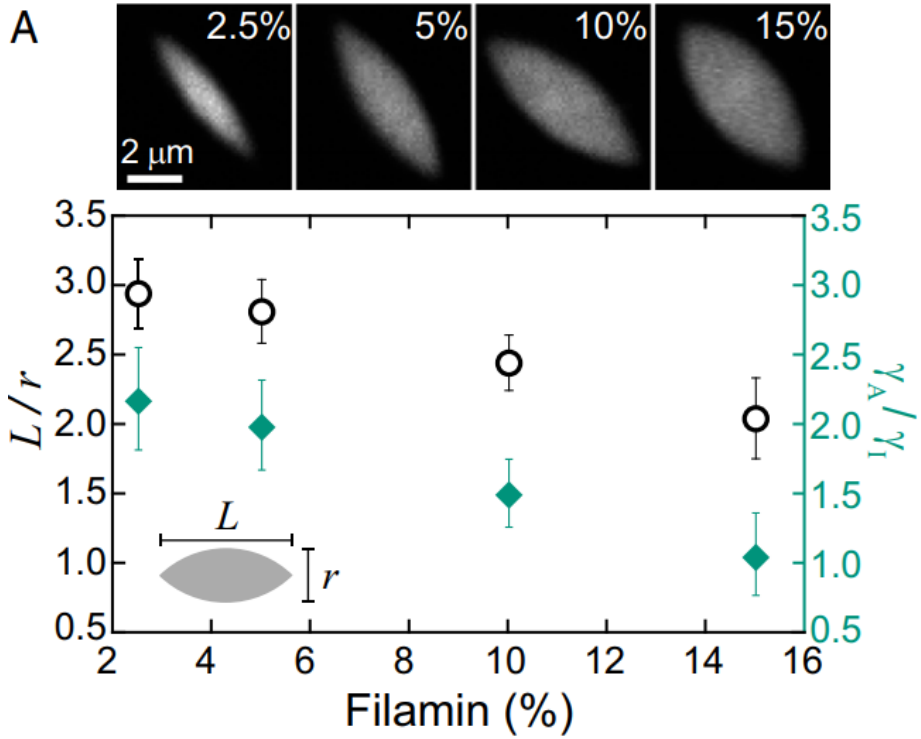
L/r vs Time


Length / Width
Time (steps)
0
0.5
1
1.5
2
2.5
3
1×10^9
2×10^9
3×10^9
4×10^9
5×10^9
6×10^9
7×10^9
8×10^9


Aspect Ratio vs Energy
Aspect Ratio (L/r)
Energy (kT)
2.5
2
1.5
1
0.5
0.6
0.7
0.8
0.9
1
1.1
1.2

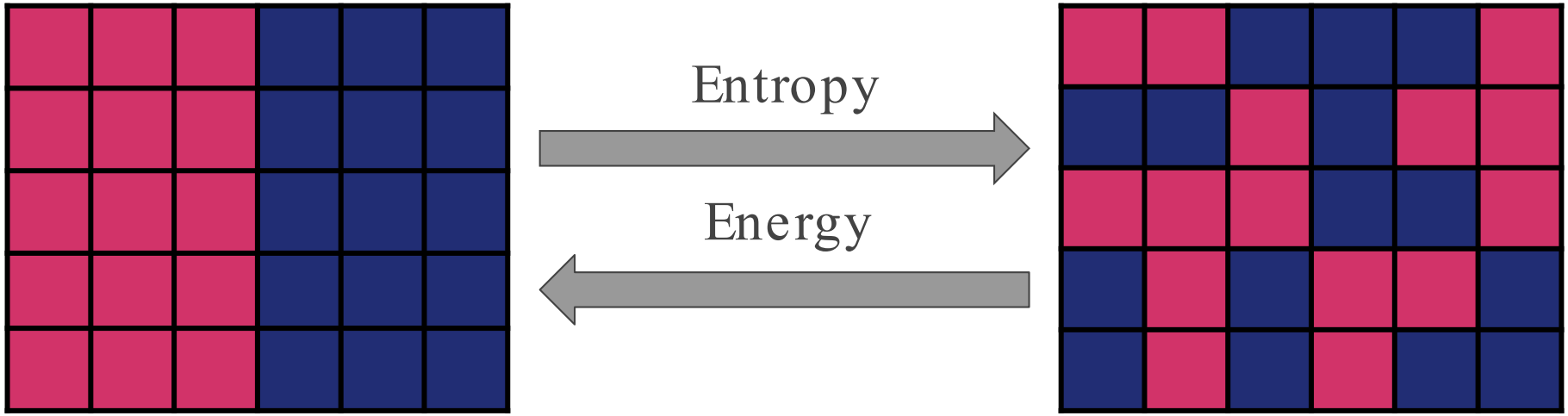
Experimental Results

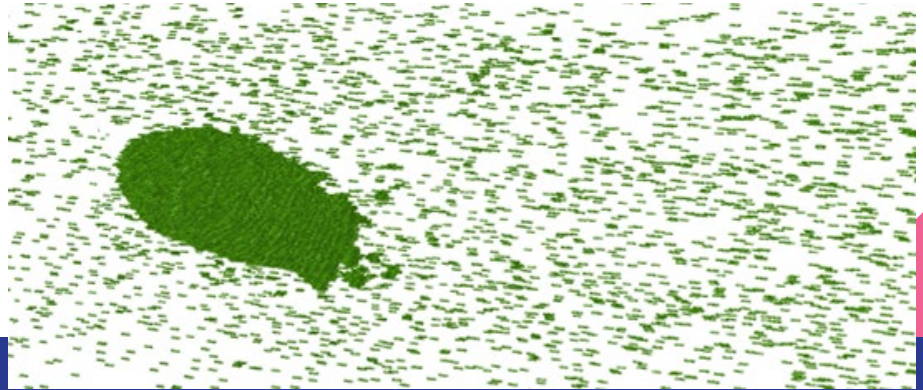




"Liquid Behavior of cross-linked actin bundles" Weirich et al.

Balance of Energy and Entropy



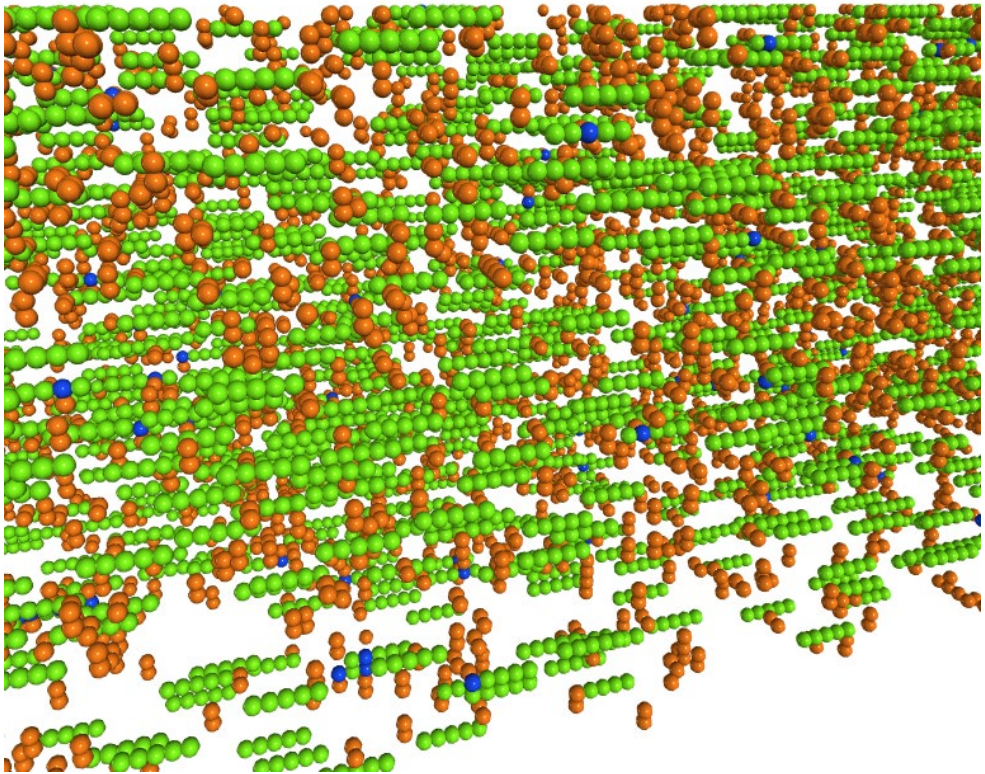


Conclusions

Still analyzing data and waiting for the second simulation

There is a difference in aspect ratio depending on the bond energy

There is a fine balance between energy and entropy



Acknowledgements

REU Organizers

Dr. Bret Flanders

Dr. Loren Greenman

Research Group

Dr. Jeremy Schmit

Tien Phan

Other Thanks

Kansas State University

National Science Foundation