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## Dynamic Monte Carlo Modeling of Protein-DNA Interactions

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# Dynamic Monte Carlo Modeling of Protein-DNA Interactions

— Aaron Kirchman —



# Background

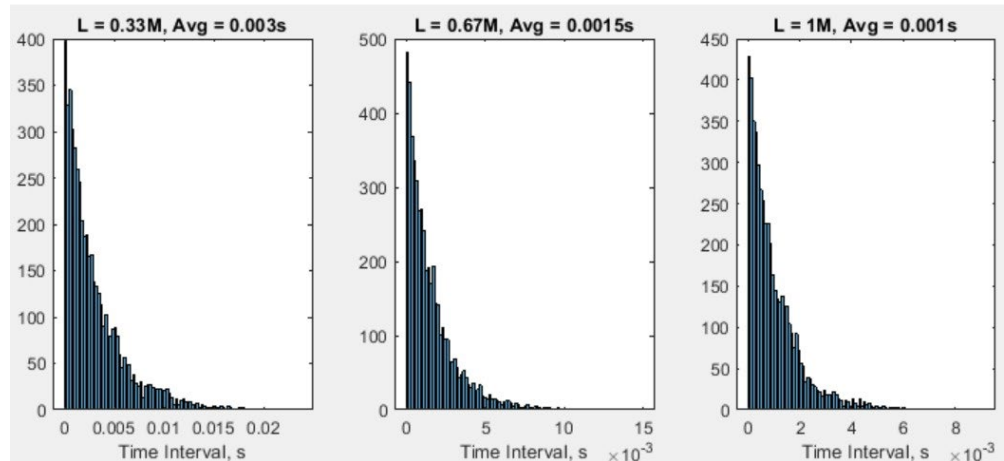
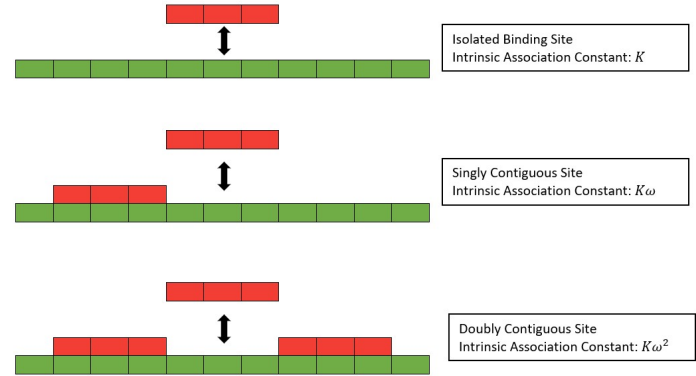
- **Simulating the real-time dynamics of interactions between nucleoproteins and DNA**
  - RAD51 dynamics on single stranded DNA
  - DNA repair
- Issues with repair or overactivity of homologous recombination (repairing DNA by combining strands) can cause cancer
- Simulation is necessary to test future hypotheses



By Conway, A.B., Lynch, T.W., Zhang, Y., Fortin, G.S., Symington, L.S.,  
Rice, P.A. - RCSB Protein Data Bank, Attribution,  
<https://commons.wikimedia.org/w/index.php?curid=19171515>

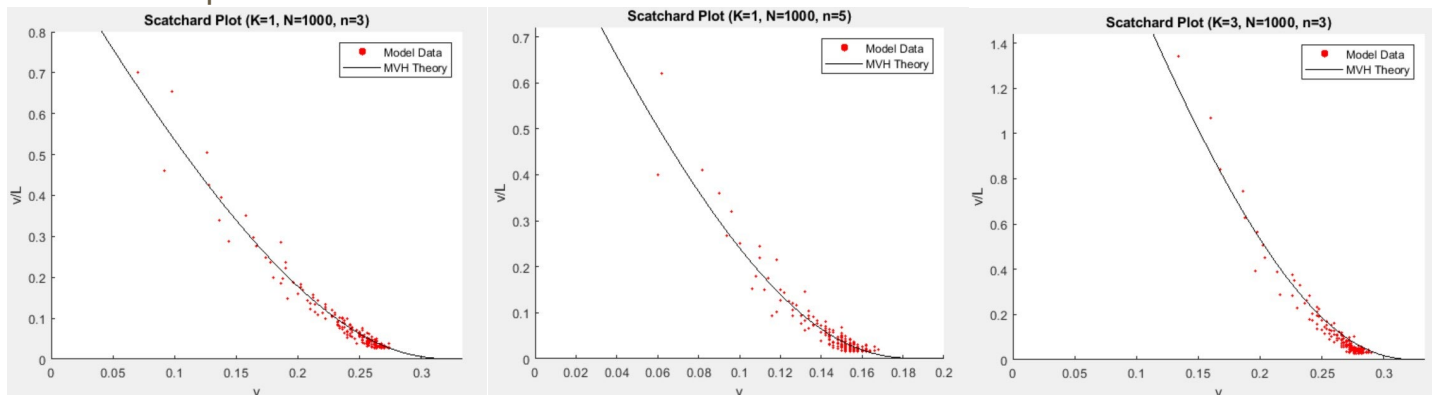
# Methods

- One Dimensional DNA Lattice
- Cooperative & Non-Cooperative Binding
- Dynamic Monte Carlo
  - Gillespie Algorithm



# Data

- Matching model to benchmark theoretical values from McGhee & von Hippel (1974)
  - Non-Cooperative



Scatchard  
Fit Values

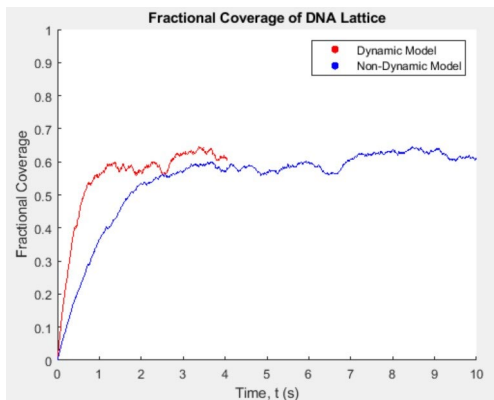
$K = 1.027$   
 $n = 3.041$   
R-Square: 0.9667

$K = 1.071$   
 $n = 5.064$   
R-Square: 0.9328

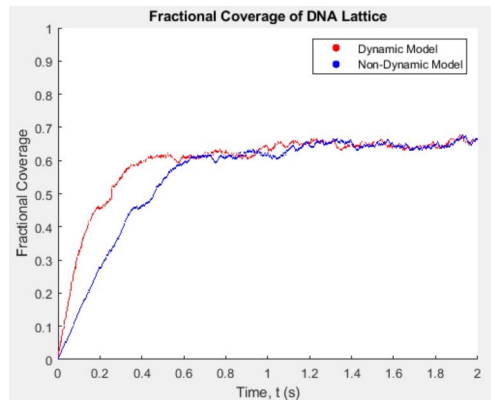
$K = 3.48$   
 $n = 3.111$   
R-Square: 0.9745

# Data

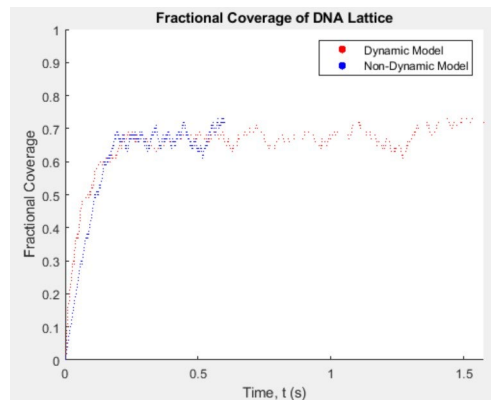
- Dynamic Monte Carlo model provides stochasticity for real-time dynamics



$N = 1000$   
 $n = 1$   
5000 Events



$N = 1000$   
 $n = 3$   
1000 Events



$N = 1000$   
 $n = 10$   
300 Events



# Future Work

- Cooperative proteins in dynamic model
- Use simulation to test hypotheses
  - Compare data from experiments
- Input RAD51 parameters

# References

- McGhee, J. D., & von Hippel, P. H. (1974). Theoretical aspects of DNA-protein interactions: Co-operative and non-co-operative binding of large ligands to a one-dimensional homogeneous lattice. *Journal of Molecular Biology*, 86(2), 469–489. [https://doi.org/10.1016/0022-2836\(74\)90031-x](https://doi.org/10.1016/0022-2836(74)90031-x)
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- van der Heijden, T., & Dekker, C. (2008). Monte Carlo Simulations of Protein Assembly, Disassembly, and Linear Motion on DNA. *Biophysical Journal*, 95(10), 4560–4569. <https://doi.org/10.1529/biophysj.108.135061>

