Simulating the Aggregation of Globular Protein in Solution at Various Salt Concentrations

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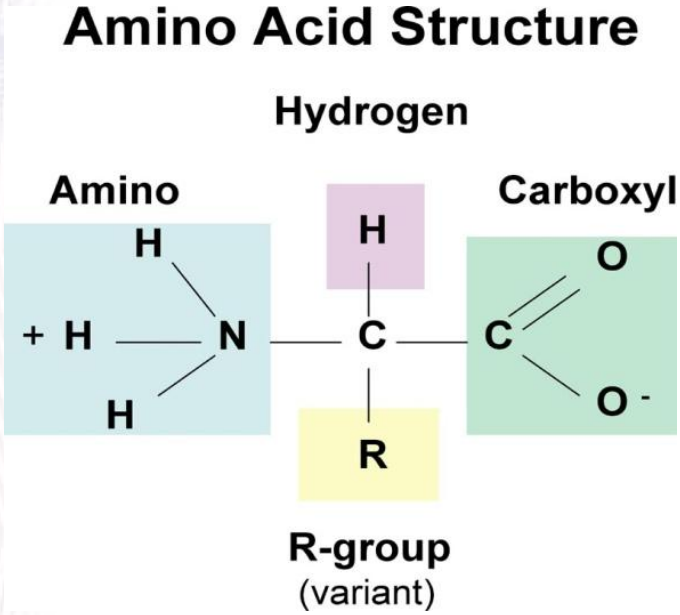
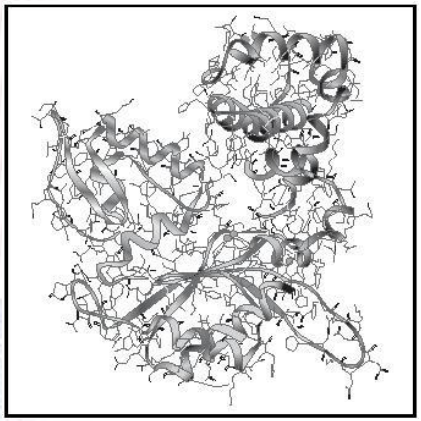
Proteins





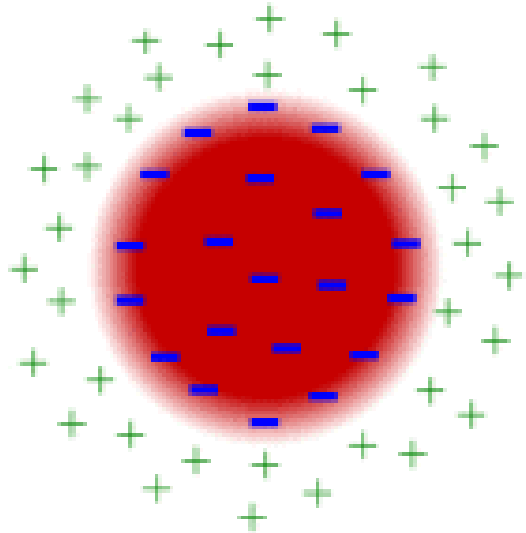
- Linear polymers of amino acids which compose a peptide chain
- Globular-have a folded chain

My Proteins

- Spherical
- 3-4 nm in diameter
- Uniform surface charge distribution

My Project

- To study the kinetic and aggregation of these proteins in solution and what happens as you vary the salt concentration
- Use the condition of constant temperature and number of proteins since those conditions are similar to those of the human body



Applications worth exploring

- Insulin delivery
- Eliminate diseases
- Destroy bacteria

Equations

- Modified Lennard-Jones Potential

$$V(r) = \frac{4\epsilon}{\alpha^2}\left(\frac{1}{(r^2-1)^6} - \frac{\alpha}{(r^2-1)^3}\right)$$

- Yukawa Potential

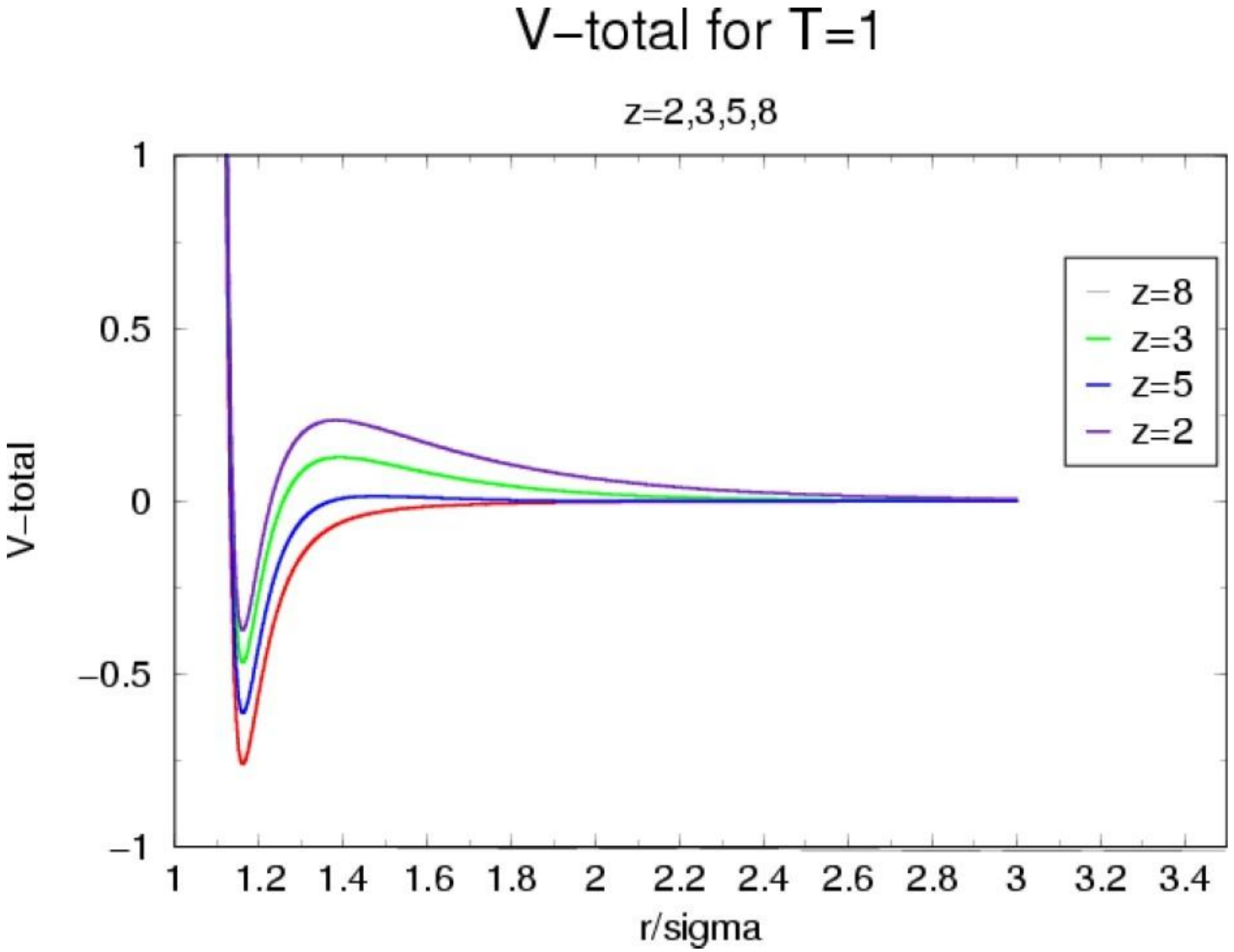
$$V(r) = A\frac{e^{-kr}}{r}, \quad 0 < r < r_{cutoff}$$

- Brownian Equation of Motion

$$\ddot{\vec{r_i}} = -\vec{\nabla}U_i - \Gamma\dot{\vec{r_i}} + \vec{W_i}(t)$$

ε-relative potential well depth
α-relative potential well width
A-relative surface charge distribution
Γ-damping coefficient

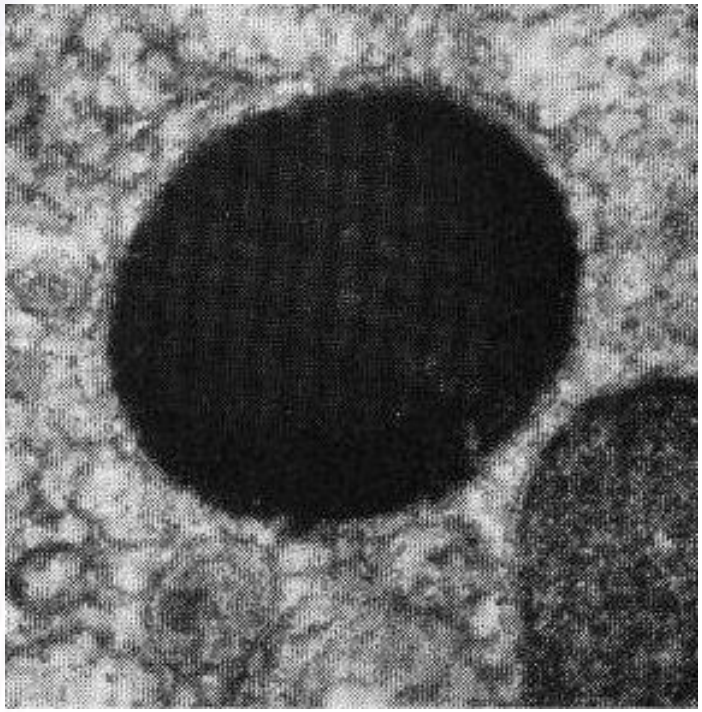
Potential Plot

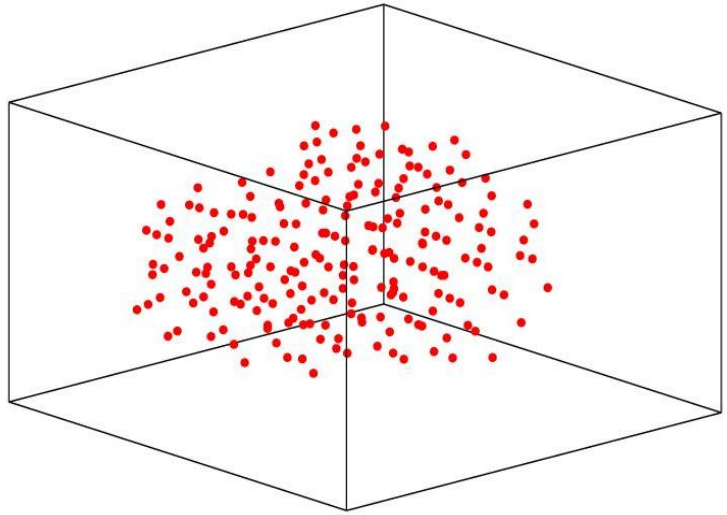


Other Similar Potentials

- DLVO Potential
- Asakura-Oosawa Potential

Lysozyme





Aggregation

- Diffusion Limited Cluster Aggregation (DLCA)
  - Stingry, fractal aggregates
  - Fractal dimension of 1.8

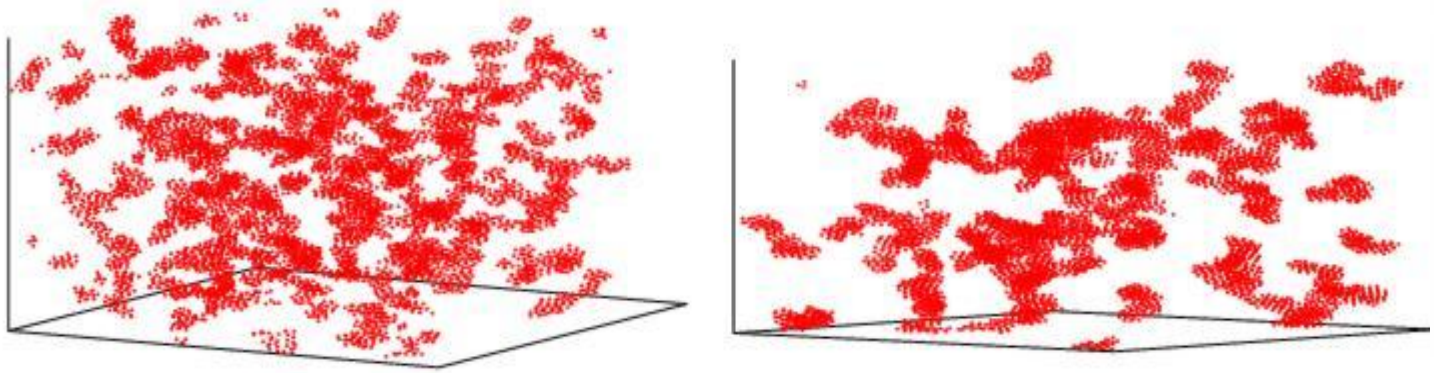
Reaction Limited Cluster Aggregation(RLCA)

Fatter cluster

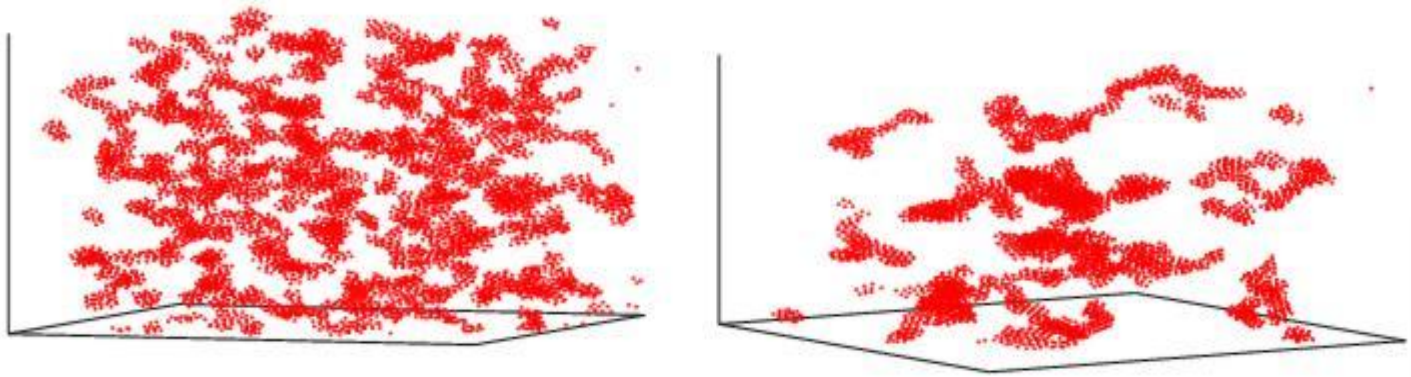
Fractal dimension of 2.1

Snapshots

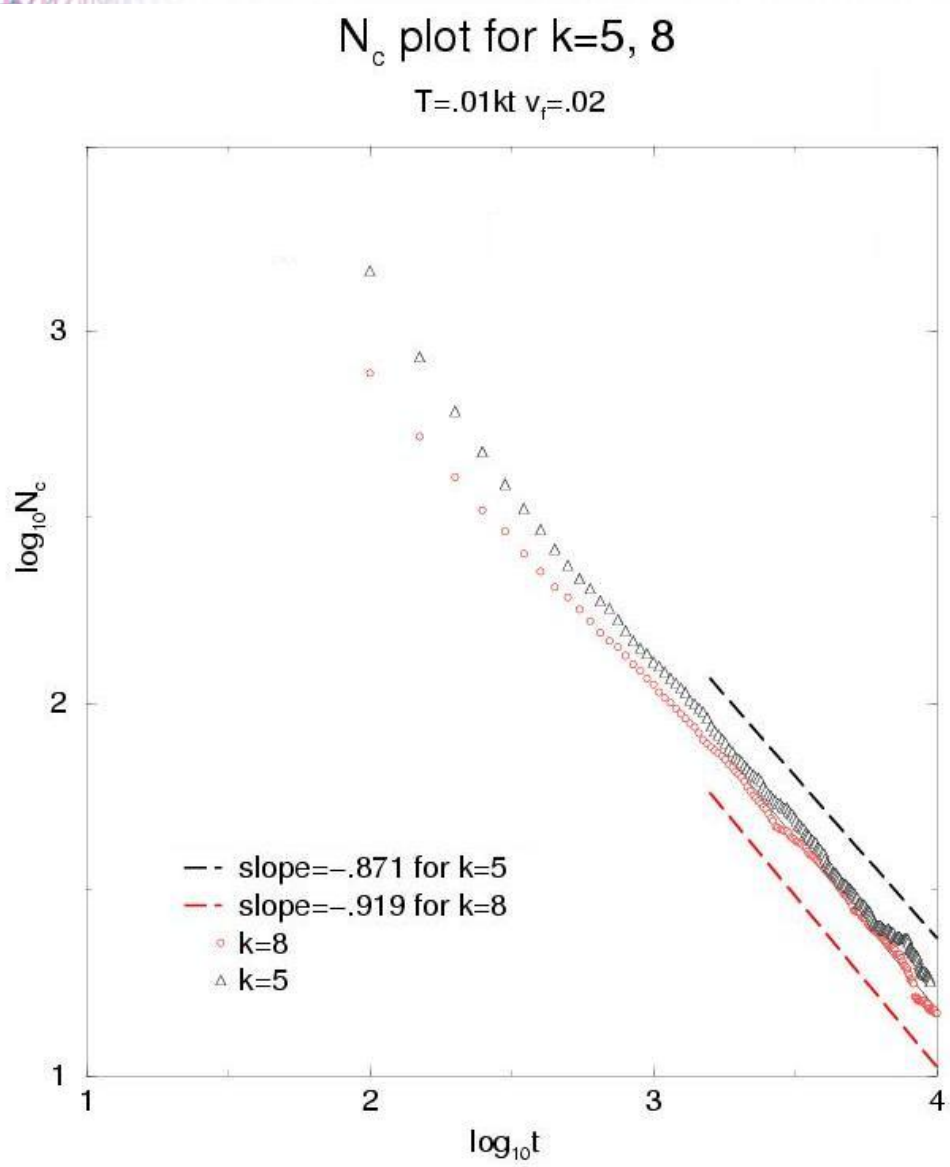
- K=5

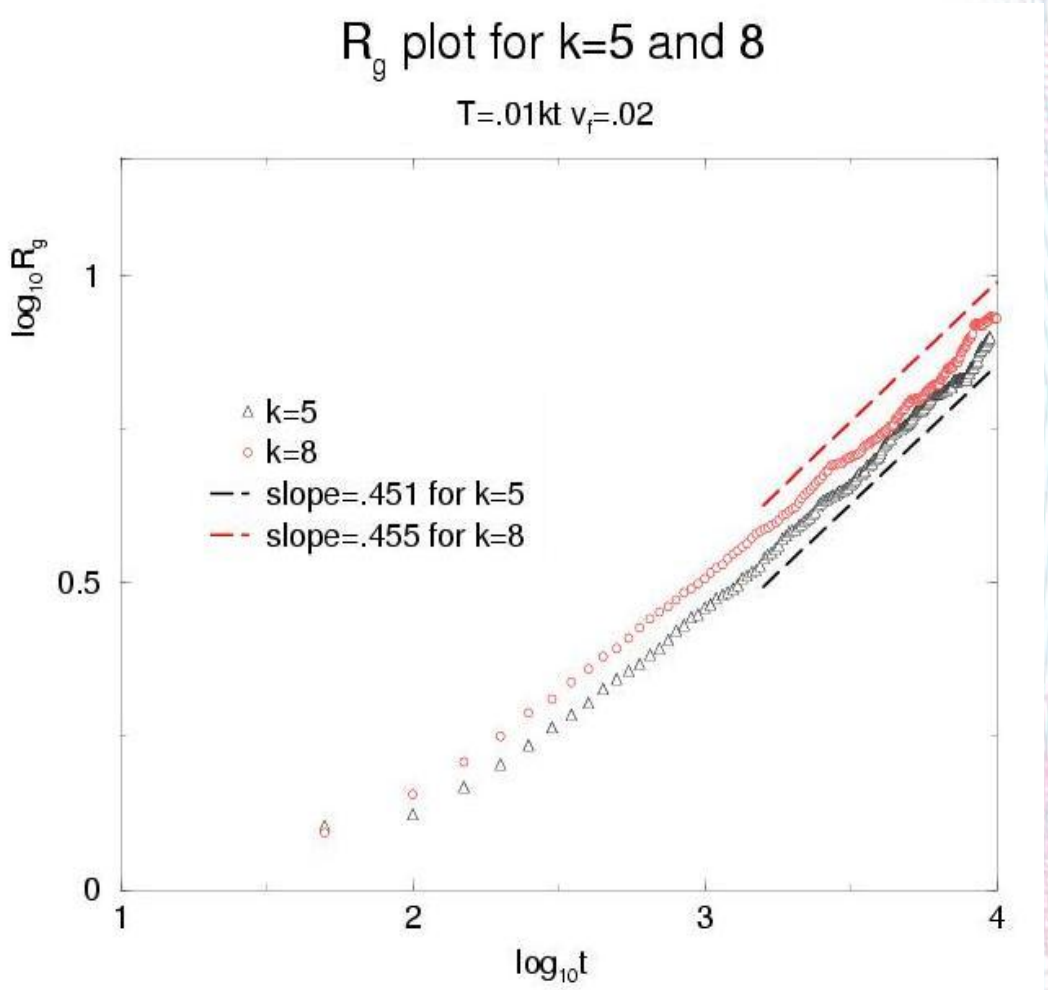


- K=8



Analyzing Data





Overall Assessment

- Took a while to get programs to work properly
- Obtained reasonable date that is physically proper
- Got a good feel for how this system works under various concentrations!

Future

- Nucleating cluster with at concentrations that have a potential barrier
- Include patchy interactions since the charge distribution of proteins is actually non-uniform

Acknowledgements

- Siddique Khan for helping me with the programming and with advice on my simulations
- Dr. Amit Chakrabarti and Dr. Chris Sorrenson for all their advice on my simulations
- ALL OF YOU FOR COMING !!!

Sources

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