Simulating the Diffusion of Nanoparticles through Physical Hydrogels

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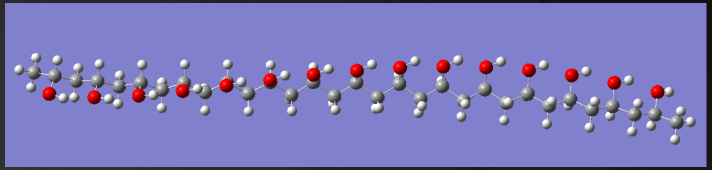
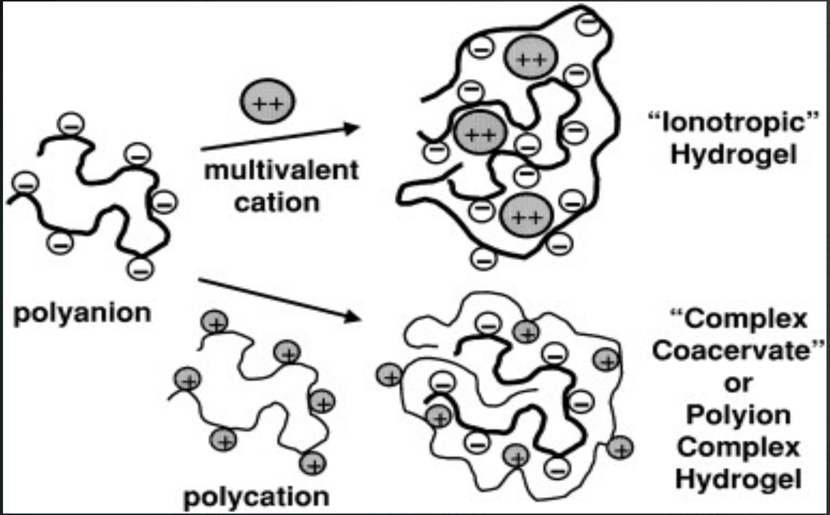
What are Hydrogels?

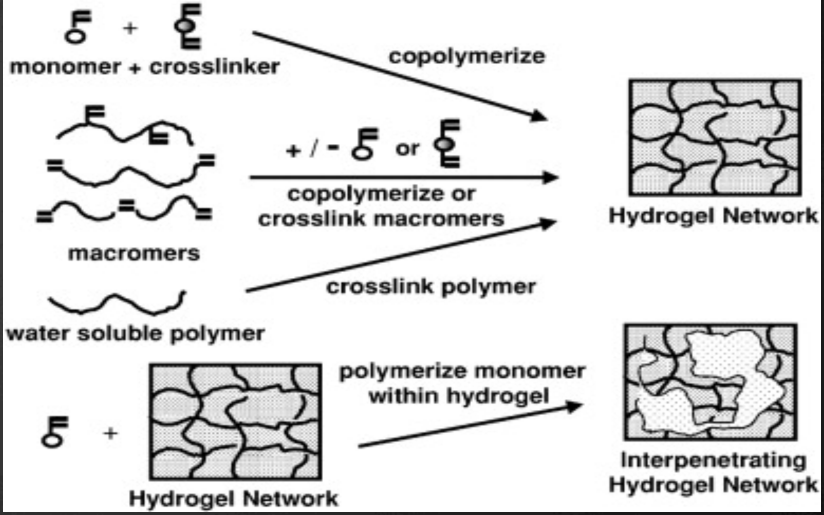
- Polymer networks → Physical and chemical



- Physical Hydrogel



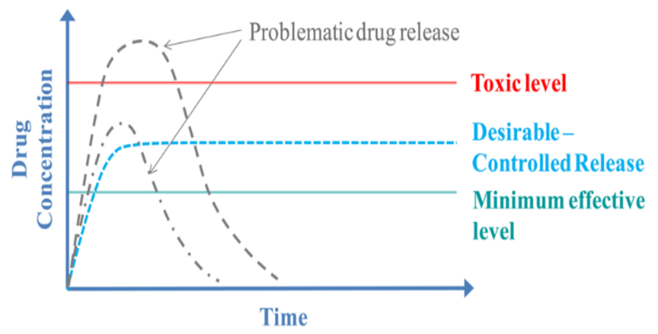
Chemical Hydrogel

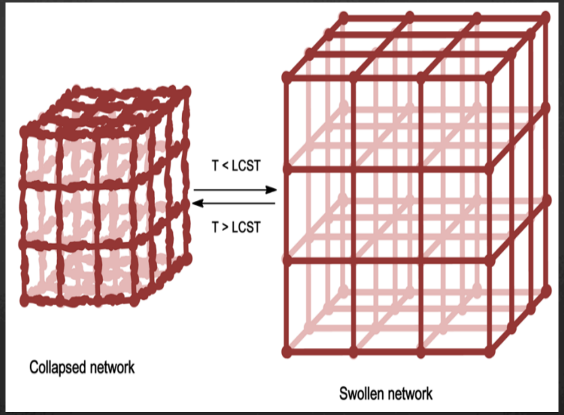


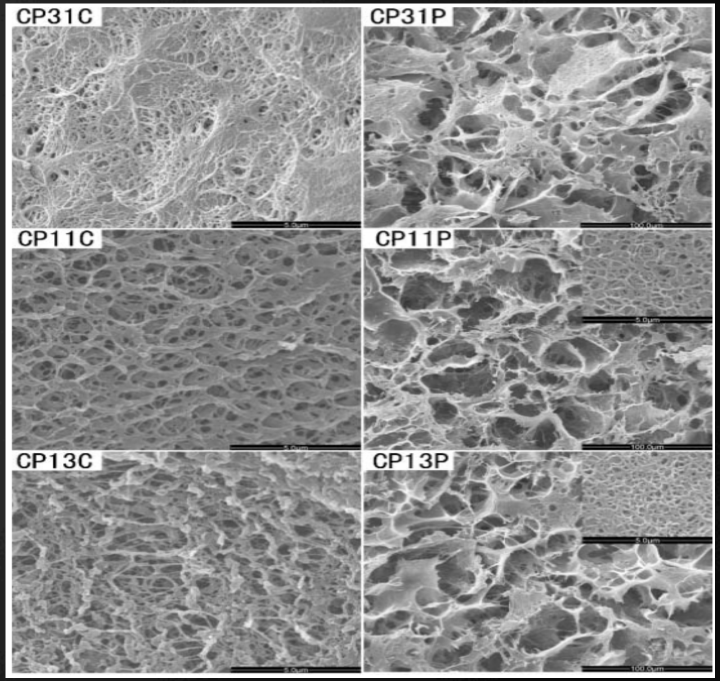
Inhomogeneous → chain entanglements, ionic interactions, points of higher or lower crosslink density (affects swelling)

Applications

- Drug Delivery (allow for tailored drug release & optimal use of the therapeutic index)







- Cell Encapsulation
- Tissue Scaffolding
- Gene Delivery

Motivation

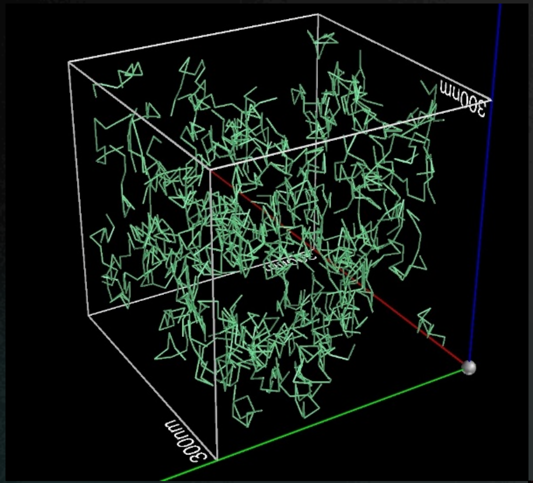
Create a computational model for tracking nanoparticles (NPs) through a physical hydrogel

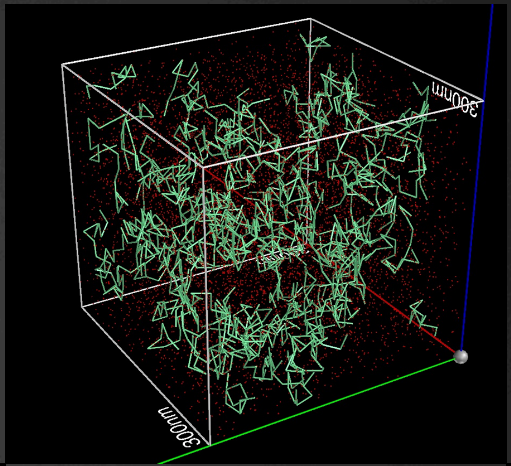
Develop an understanding of the various contributions (energy) to the diffusion of NPs through a polymer network

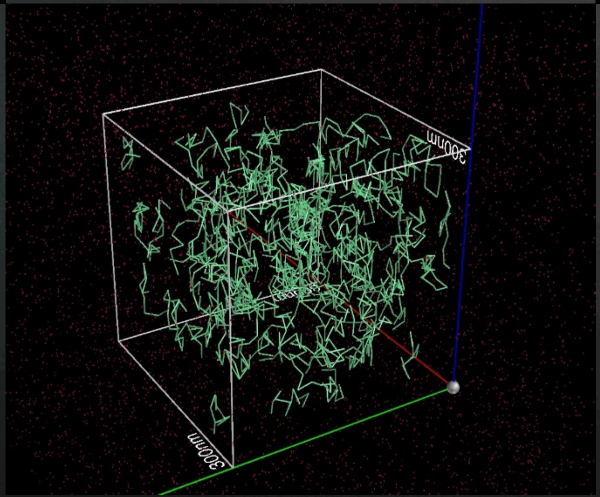
Methodology

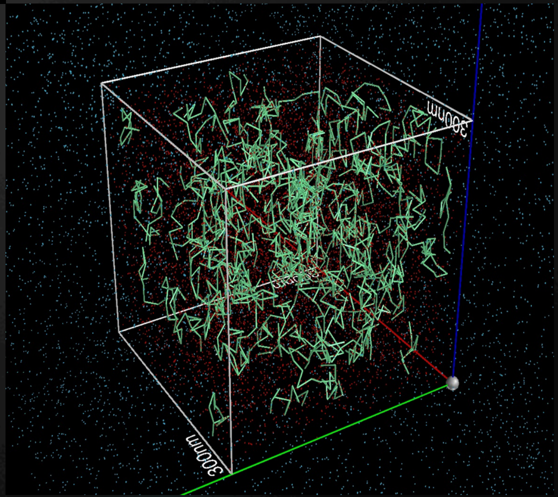
- Random walk Monte Carlo algorithm used to determine energetically favorable NP/polymer moves as hydrogel swells or contracts
- MATLAB used to simulate the diffusion through a 1 μm^3 partitioned box containing a physical hydrogel.
- Van der Waal & Columbic interactions
- Java code (Ben Beach) for visualization
- Hydrodynamic radius of the NPs & polymers considered
- Hydrogel is generic physical hydrogel
- If a proposed move lowers the energy, it is accepted
- If not, accounting for thermal energy, the move is accepted with Boltzmann probability

Java Visualization

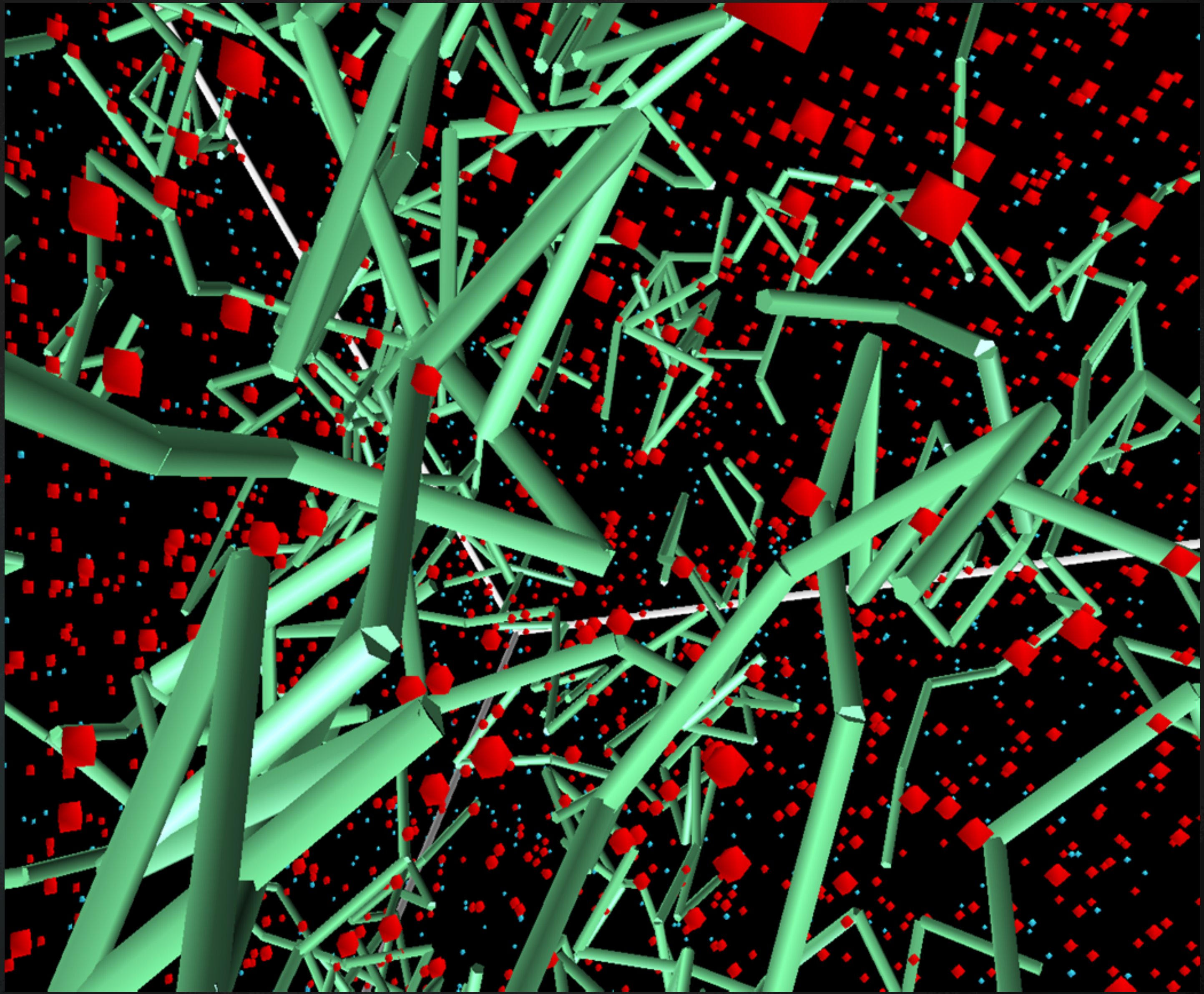






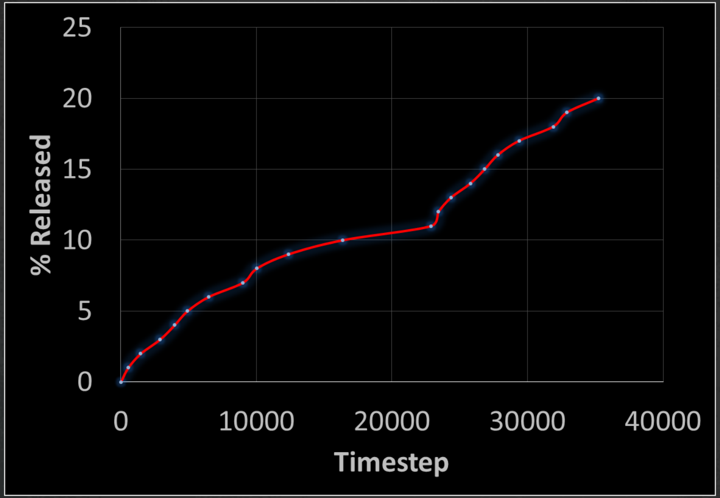


More…



Results & Conclusions

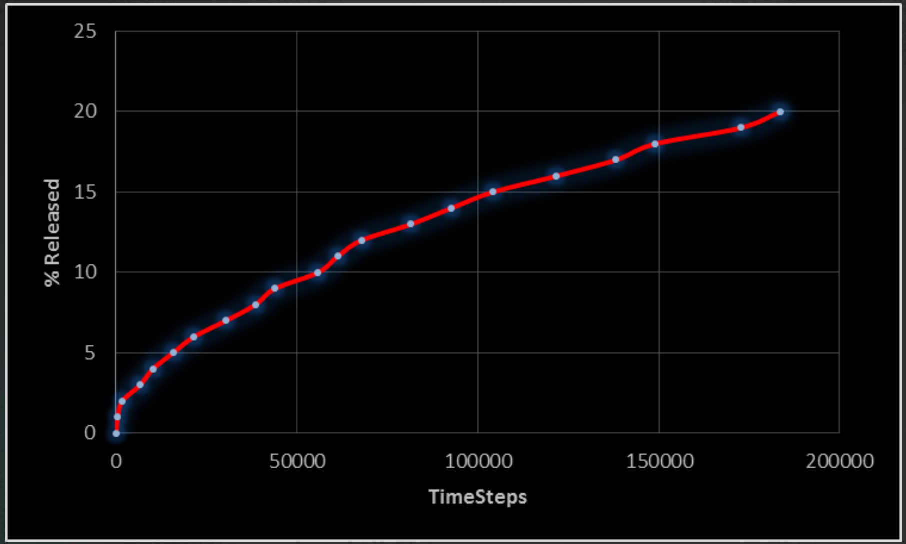
- Successful creation of a 3-D course grain Monte Carlo model Case studied →



- The hydrogel expands the particles are released and the hydrogel expands again.
- Not realistic but slope signifies change in diffusion rate

Results and Conclusions, cont…

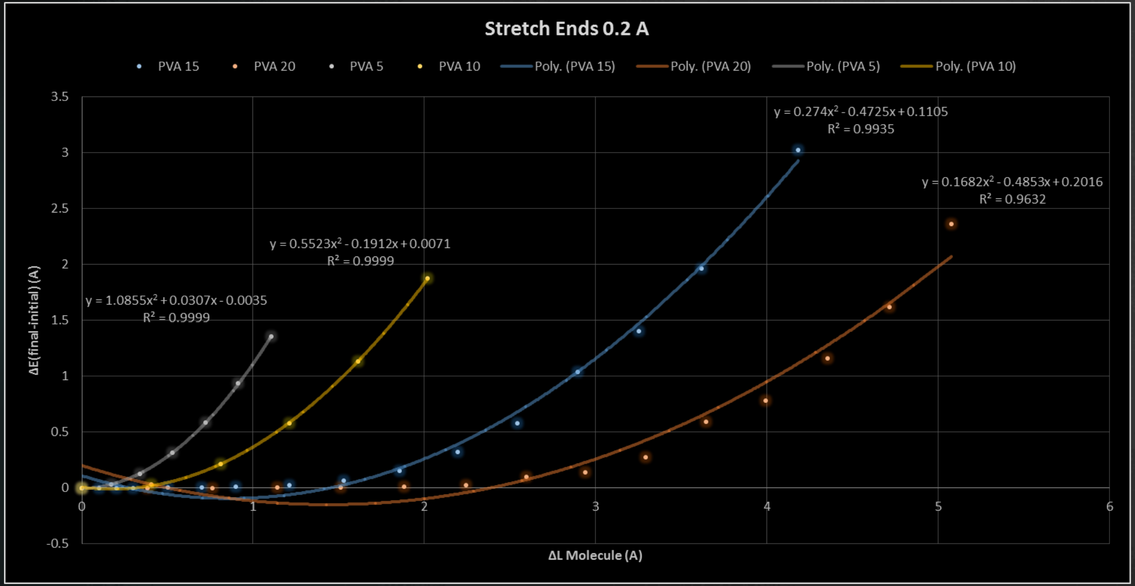
- Case 2 → Concurrent transition/ motion of polymer strands and NPs

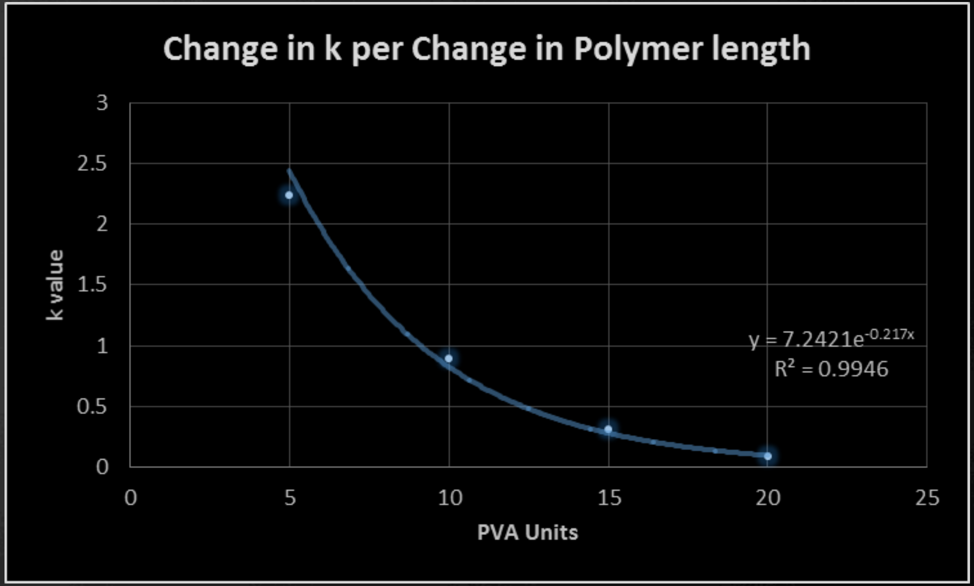


- Model is a promising alternative to the computationally intensive molecular dynamics approach to simulating diffusion

Most Recently

- Trying to determine an approximate spring constant value for PVA polymer strands
- Elastic energy to be used for a more realistic change in size of the hydrogel





Future Work

- Validate simulations with experimental data
- Build a model for cross-linked hydrogels
- Extend model to take into account external fields
- Derive coefficients such as the molecular weight between crosslinks. M_C, and calculate how changes in them influence the diffusion process

Acknowledgements

- Dr. Pedro Derosa
- All the students, graduate and undergraduate in my lab.
- Dr. Ramu Ramachandran
- Lindsay Gouedy
- Jessica Wasserman

LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

The End

- Thank you for your time and this opportunity


ANY
QUESTIONS
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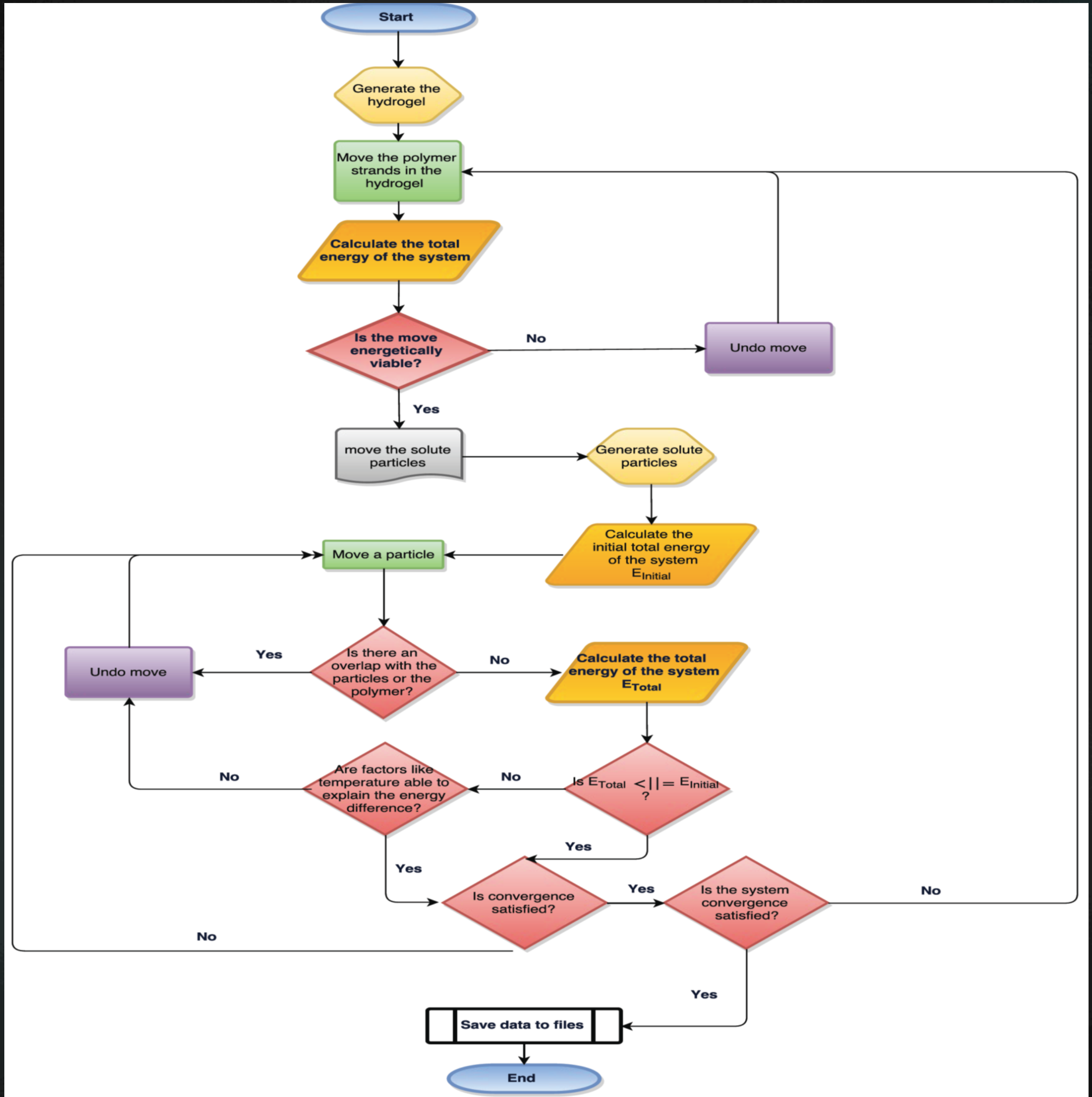
Start
Generate the hydrogel
Move the polymer strands in the hydrogel
Calculate the total energy of the system
Is the move energetically viable?
No
Undo move
Yes
move the solute particles
Generate solute particles
Calculate the initial total energy of the system $E_{Initial}$
Move a particle
Is there an overlap with the particles or the polymer?
Yes
Undo move
No
Calculate the total energy of the system E_{Total}
Is E_{Total} < || = $E_{Initial}$?
No
Are factors like temperature able to explain the energy difference?
No
Yes
Yes
Is convergence satisfied?
Yes
Is the system convergence satisfied?
No
No
Yes
Save data to files
End