Development of a Dissipative Particle Dynamics framework for simulating tetra-PEG gels with degradable crosslinks

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Motivation
Biomedical applications of controllably degradable tetra-PEG gels

Directed growth of neural networks using degradable gels

Goal: Develop a coarse-grained numerical framework for simulating degradation in gels

Method – Updated Implementation
Loop over N timesteps
fix=initial_integrate();
fix_post_integrate();
nflag=neighbor->decide();
if nflag:
fix->pre_neighbor();
neighbor->build();
fix->post_neighbor();
else:
fix->pre_force();
force->compute();
fix_post_force();
fix->final_integrate();

Validation
Overlap with analytical:
\[ \frac{N}{N_0} = \exp(-kt) \]

Swelling without degradation

Chain length distribution in swollen gels

Fragment size evolution analysis: fragment size – # of beads

Conclusions and Future work
✓ Initial framework for simulating degradable gels
✓ Control over degradation rate
✓ “Reverse gelation” vs. surface erosion
✓ Introduce reversible bonds

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