Motivation
- Actin filaments, or microfilaments, are long (~ several μm), double-stranded, helical filaments that span the cytoplasm of cells.
- Typical diameter only ~6 nm across, but have a pitch length (distance for one full “twist” of double helix) of ~72 nm.¹
- Important for cell mobility and cell division, but assembly mechanism still not well understood.
- How do we make double-stranded helical structures that mimic microfilaments such that we can study the self-assembly process?

Model to replicate F-actin geometry
- Rigid bent-rod monomers (core sites + attractive sites)
- Vertical bonding builds protofilaments while staggered lateral bonding links helices together
- Protofilaments have 12 monomers (n=12) per pitch; ideal filament/protofilament has at least 1 full pitch
- Bonding interactions only between attractive sites in the same color using soft cosine potential² – varying binding strength A leads to various structures

\[ U(\varphi) = -A \left[ 1 + \cos \left( \frac{\pi \varphi}{\varphi_0} \right) \right] \]

Various self-assembled structures

Self-assembly structural diagram and assembly kinetics
- Double-stranded actin-like filaments are formed when \( A_S \) and \( A_D \) are in the appropriate range (green zone in the structural diagram). Self-assembly mainly proceeds via an addition polymerization scheme: one monomer is added at a time. However, we also find oligomer addition and filament merging, though rarely.

Why are actin filaments double-stranded?

Why do actin filaments seem to have \( A_S > A_D \)?

Various structures are obtained by varying \( A_S \) and \( A_D \).

References

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