Biopolymer networks

Biopolymers such as actin, cellulose or chitin are macromolecules synthesized by living organisms in order to carry out various essential tasks. In many cases, these molecules establish networks. The most versatile among these networks is the protein backbone of the cell, the cytoskeleton (Fig. 1a, green):

**Components:**
- Actin, intermediate filaments, microtubules
- Support/initiate cell division/migration/motility
- Mechanotransduction, etc.

**Functions / tasks:**
- Maintain mechanical stability
- Support/initiate cell division/migration/motility
- Mechanotransduction, etc.

Very little knowledge about network mechanics

Experiments have limits that simulations do not: capturing events on subcellular length and time scales very demanding, often impossible

**Finite Element Approach**

- Filaments \(\rightarrow\) Beam Elements, excellent match to experiments and theory [7]
- Stochastic forces and moments (molecule collisions): **Space-time white noise**

\[
\begin{align*}
\mathbf{f}_{\text{stock}} &= \sqrt{2k_B T s_{\text{str}} n} \frac{\partial W_f(x(t))}{\partial x(t)} \\
\mathbf{m}_{\text{stock}} &= \sqrt{2k_B T s_{\text{rot}} n} \frac{\partial^2 W_m(x(t))}{\partial x(t)^2}
\end{align*}
\]

- Dynamics modeled by **stochastic partial differential equations (SPDEs)**

\[
\begin{align*}
\mathbf{f}_{\text{ext}}(x, \theta, \xi, t) + \mathbf{f}_{\text{visc}}(x, \theta, \xi, t) &= \mathbf{f}_{\text{ext}}(x, \xi, t) + \mathbf{f}_{\text{visc}}(x, \xi, t) \\
\mathbf{m}_{\text{ext}}(x, \theta, \xi, t) + \mathbf{m}_{\text{visc}}(x, \theta, \xi, t) &= \mathbf{m}_{\text{ext}}(x, \xi, t) + \mathbf{m}_{\text{visc}}(x, \xi, t) + \alpha'(\xi) \times \mathbf{q}_{\text{ext}}(x, \theta, \xi, t)
\end{align*}
\]

- Mathematical intricacies of SPDEs require care with discretization / integration

\(\rightarrow\) Finite element discretization in space, backward Euler scheme in time [7,8].

\(\rightarrow\) Discrete, piecewise constant stochastic forces and moments

**Simulation of cytoskeletal polymorphism**

**Investigate the cytoskeleton’s ability to shift shapes**

**Setup:**
- Periodic boundary conditions
- **Point-like crosslinkers**, subject to diffusion (Fig. 2)
- Links establish by evaluating binding potentials
- Constraints for Linkers connecting two filaments:
  - Proximity and inter-filament orientation
  \(\rightarrow\) if constraints met, add element

**Result:** Vary linker species/conc. \(\rightarrow\) different network types (Fig. 4); observed in experiments (Fig 1b,c) [2-5].

**Future work**

- Include contact for very slender structures
- Efficient contact detection: Octree & OBBS
- Modeling binding spot geometry: actin double-helix
- Modeling of crosslinker power stroke

**REFERENCES:**