

SI Text

Cytoskeletal Dynamics Simulation. The dynamic simulation presented in this work is based on the Newton's equations of motion.

$$m_i \frac{d^2 \mathbf{r}_i(t)}{dt^2} = \mathbf{f}_i \equiv -\frac{\partial U}{\partial \mathbf{r}_i}, \quad [1]$$

where $i = 1, 2, \dots, N$, $\mathbf{r}_1(t), \mathbf{r}_2(t), \dots, \mathbf{r}_N(t)$ are the positions of N interacting particles and $U = U(\mathbf{r}_1(t), \mathbf{r}_2(t), \dots, \mathbf{r}_N(t))$ is the potential energy of the many-body system. It is known that closed Newtonian systems conserve the total energy and hence in the framework of equilibrium statistical mechanics they correspond to the microcanonical ensemble which is characterized by constant total energy E , constant number of particles N and constant volume V . Biological systems however, usually operate at a constant physiologically relevant temperature of approximately 300 K and therefore they are better described by the canonical ensemble, which is characterized by constant number of particles N , constant volume V and constant temperature T . Our cytoskeletal dynamic simulation was performed in the context of the canonical ensemble.

In our coarse-grained simulation, the removal of water and other degrees of freedom should introduce viscous dissipative forces and corresponding thermal fluctuation forces on the coarse degrees of freedom. These forces will in principle have spatial-temporal memory kernels (generalized Langevin equation and hydrodynamic coupling). The details of the implementation will influence the value of τ_g . However, we chose not to pursue this in our first paper on remodelable cytoskeleton. The reason is that there are gross uncertainties in the biochemical details of the kinetics of protein-protein dissociation and re-association, and the fact that these processes could be enzyme catalyzed. With these uncertainties present, the improvement brought by solving the generalized Langevin equation is less significant, while the computational cost would increase greatly. We believe the physics revealed in the coarse-grained simulation above timescale τ_g is generic.

The Berendsen Thermostat. The Berendsen algorithm (1) was employed to regulate the initial low temperature towards the desired temperature of 300 K and then to maintain it constant throughout the numerical experiment. The method realizes a weak coupling of the system to an external bath being at the constant desired temperature T_f . The Berendsen thermostat is a very simple and robust technique. It is based on the equations

$$dv_i/dt = F_i/m_i + \zeta (T_f/T - 1)v_i, \quad [2]$$

where $i = 1, 2, \dots, N$, v_i is the particle velocity, F_i is the force acting on the particle, m_i is the particle mass, ζ determines the strength of the coupling to the bath and T is the instantaneous thermodynamic temperature of the system calculated by exploiting the equipartition theorem.

Virial Stress. The instantaneous total or volume averaged stress tensor in our cytoskeletal dynamics simulation was calculated using the Virial formula (2)

$$\tau_{ij} = \left\langle \frac{1}{\Omega} \hat{S}_2 \left(\sum_{N=1}^N \frac{-p_i^n p_j^n}{m_n} + q_i^n \nabla_j^n U(q^N) \right) \right\rangle, \quad [3]$$

where $\langle \rangle$ means canonical ensemble average in the original system configuration, Ω is the system volume, \hat{S}_2 is the symmetrization operator defined as $\hat{S}_2(G_{ij}) = 1/2(G_{ij} + G_{ji})$, p_i^n and q_i^n are the i components of the momentum and the position of the n -th particle, m_n is the mass of the n -th particle and U is the potential energy of the system. The above expression can be derived from the equation

$$\tau_{ij} = \frac{1}{\Omega} \hat{S}_2 \left(\left. \frac{\partial F}{\partial \eta} \right|_{equil.} \right), \quad [4]$$

where $F = E - TS$, is the Helmholtz free energy, and η is the supercell strain.

1. Berendsen, H. J. C., Postma, J. P. M., Vangunsteren, W. F., Dinola, A. & Haak, J. R. (1984) *J. Chem. Phys.* **81**, 3684-3690.
2. Lutsko, J. F. (1988) *J. Appl. Phys.* **64**, 1152-1154.