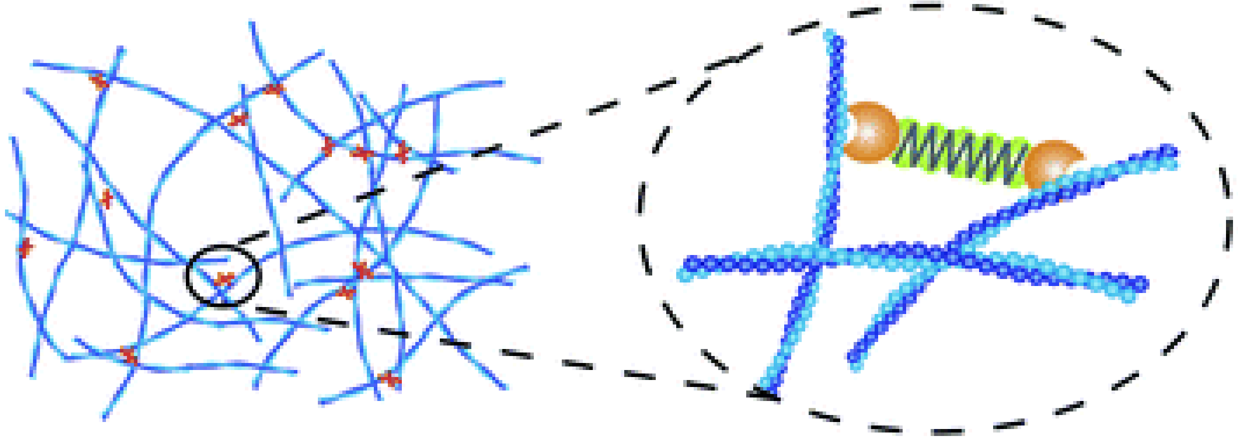
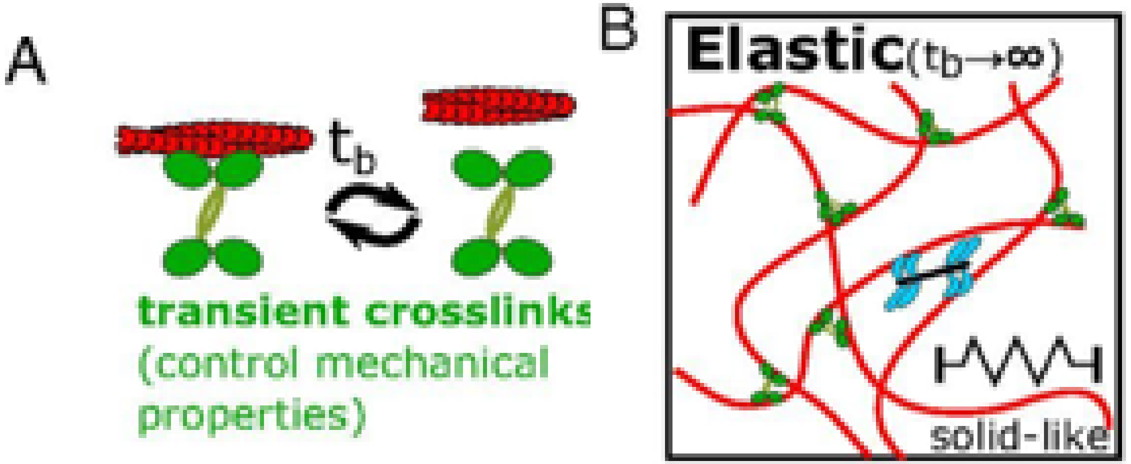
Reaction-Diffusion Modelling for the Cross-Linking of Actin Gels

KISHORE BASU, ONDREJ MAXIAN, ALEKSANDAR DONEV

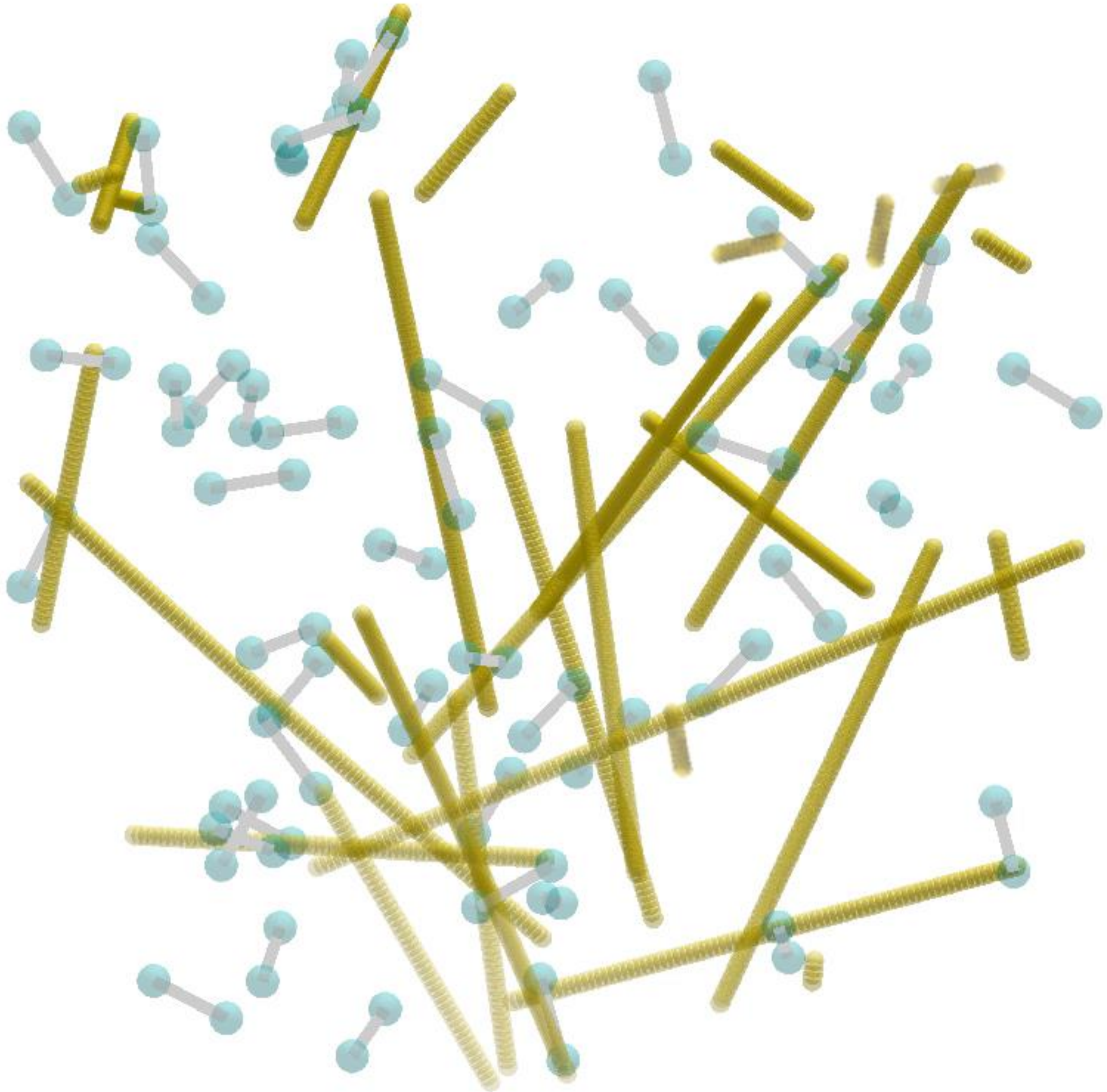
Background




A
t_b
transient crosslinks
(control mechanical
properties)
B
Elastic(t_b→∞)
solid-like

What makes this difficult:

- Theory difficult: Highly dependent on the geometry of the actin network
- Simulations difficult: Diffusion controlled, limiting step is the diffusion, not the reaction.
- Diffusion controlled → want large time step



My goal:

- Add **dimers** to reaction-diffusion code (Stochastic Reactive Brownian Dynamics) in Fortran 95
- Develop time integrator that allows large time step size

Donev, et. al. Efficient Reactive Brownian Dynamics. *J. Chem. Phys*. **148,** 034103 (2018)

How do microscopic parameters, such as the reaction rate and reaction radius, change the macroscopic properties of the cytoskeleton?

Overdamped Langevin Equation for Cross-Linkers

$\boldsymbol{r}_1$ – position of particle 1
$\boldsymbol{r}_2$ – position of particle 2
dW – white noise
k – spring constant
μ – mobility coefficient
l_0 – rest length
l – $\|r_1 - r_2\|$
k_b – Boltzmann's constant
$D = k_b T \mu$ – diffusion coeff
T – Temperature
$\boldsymbol{r}_{cm}$ – centre of mobility

$$F_i = k\,\mu_d \left(\frac{l_0 - l}{l}\right)\boldsymbol{r}_d$$

$$\mu_d = \mu_1 + \mu_2$$

$$\boldsymbol{u} = \frac{\boldsymbol{r}_1 - \boldsymbol{r}_2}{l}$$

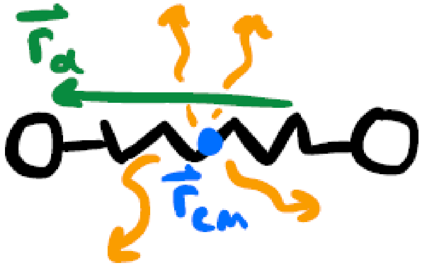
$$\boldsymbol{r}_d = \boldsymbol{r}_1 - \boldsymbol{r}_2$$

$$d\boldsymbol{r}_i = \mu_i \boldsymbol{F}_i\, dt + \sqrt{2D_i}\, d\boldsymbol{W}_i$$

$$\downarrow$$

$$d\boldsymbol{r}_{cm} = \sqrt{2D_{cm}}\, d\boldsymbol{W}_{cm}$$

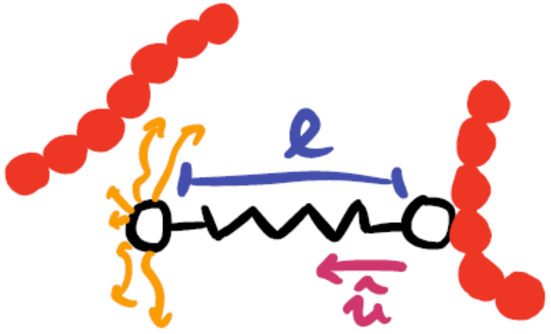
$$d\boldsymbol{r}_d = \mu_d \boldsymbol{F}_d\, dt + \sqrt{2D_d}\, d\boldsymbol{W}_d$$



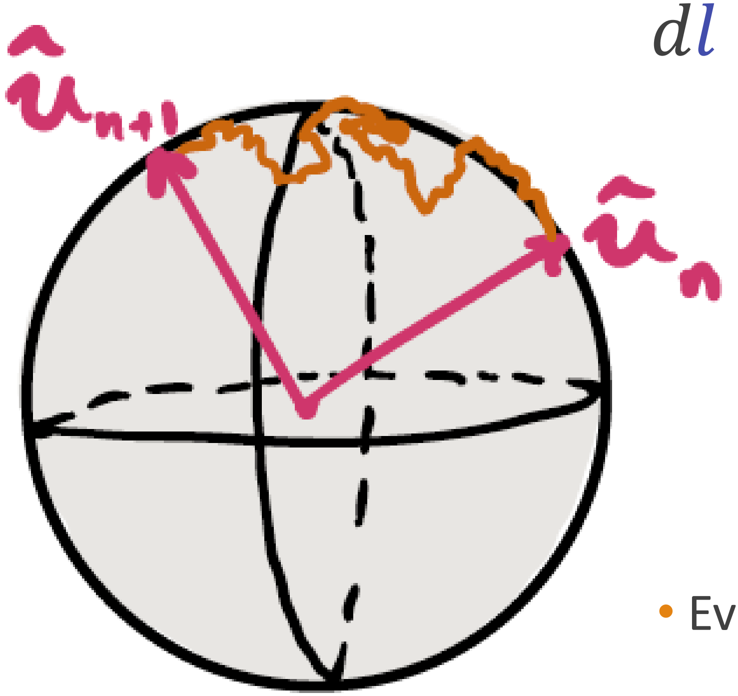
$$\downarrow$$

$$dl = \left((l_0 - l)k\mu_d + \frac{2D_d}{l}\right)dt + \sqrt{2D_d}\, dW_l$$

$$d\boldsymbol{u} = \frac{-2D_d}{l^2}\boldsymbol{u}\, dt + \frac{\sqrt{2D_d}}{l}\boldsymbol{u} \times d\boldsymbol{W}$$



Time-Marching Scheme



$$dl = \left((l_0 - l)k\mu_d + \frac{2D_d}{l} \right) dt + \sqrt{2D_d}\, dW_l$$

- Used the Implicit Trapezoidal method

$$d\boldsymbol{u} = \frac{-2D_d}{l^2}\boldsymbol{u}\, dt + \frac{\sqrt{2D_d}}{l}\boldsymbol{u} \times d\boldsymbol{W}$$

- Euler-Lie integrator
- Evolves Brownian motion on the unit sphere using rotations

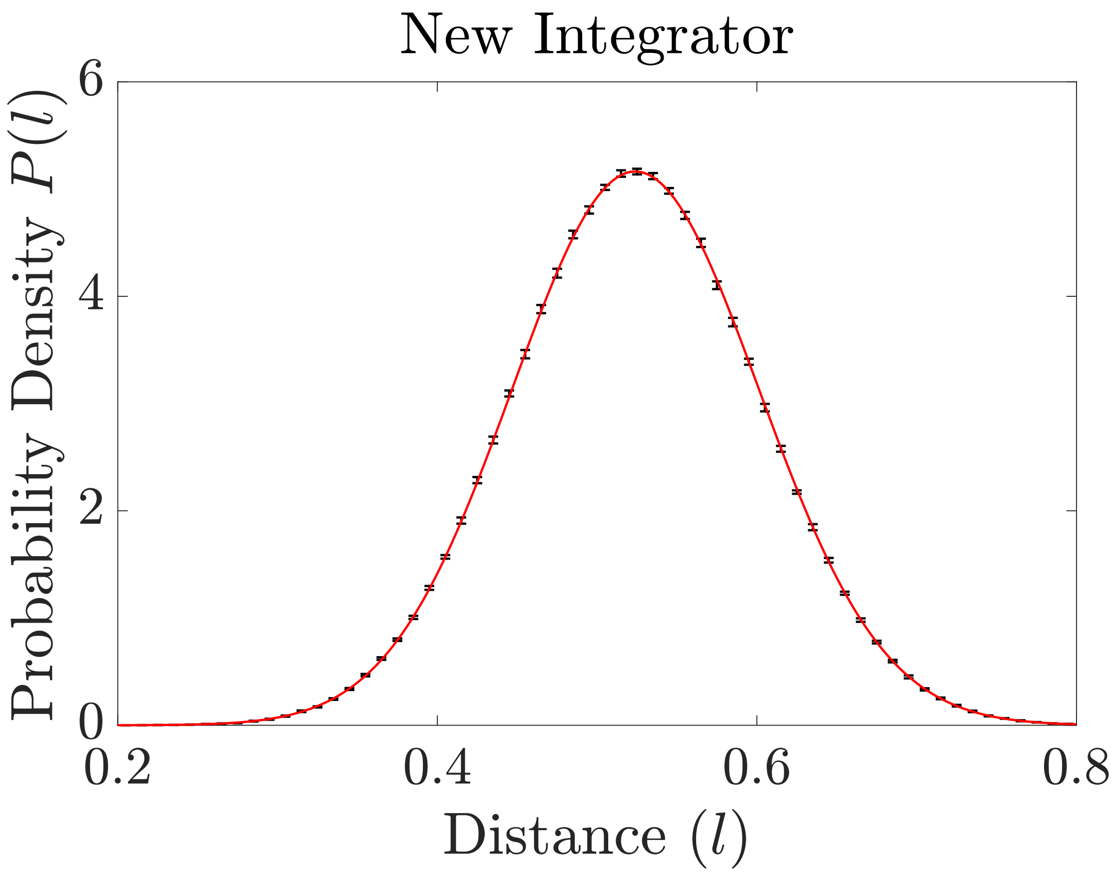
Delong, et. al. Multiscale Temporal Integrators for Fluctuating Hydrodynamics. *Phys. Rev.* E 90, 063312, 2014.

How do we know our results are correct?

Gibbs-Boltzmann Distribution

$$dP(l) = \frac{1}{Z} l^2 \exp\left(\frac{-k(l - l_0)^2}{2\, k_b T}\right) dl$$

Z – Normalizing Factor



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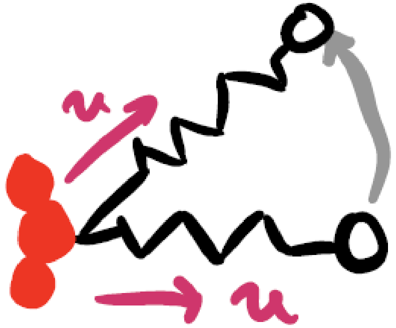
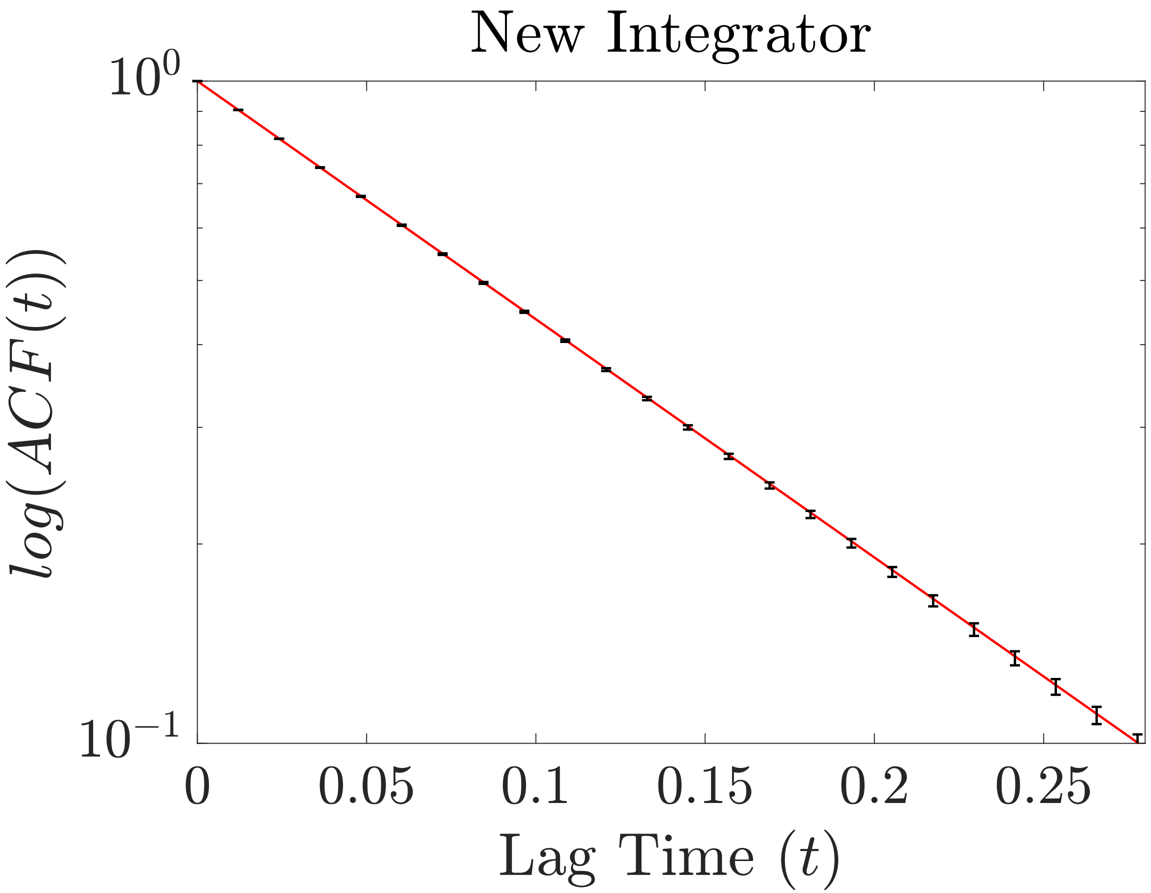


$$ACF(t) \coloneqq < \boldsymbol{u}(t+t_0) \cdot \boldsymbol{u}(t_0) >$$

$$ACF(t) = \exp(-\frac{|t|}{\tau_r})$$

$$\tau_r = \frac{l_0^2}{2D_d}$$



Future Work

- Add reverse reactions to allow for unbinding
- Measure the macroscopic rate of binding
- Real CLs are cylindrical, parallel/perpendicular mobilities