Polymer Growth Simulation

Assembly Against a Force

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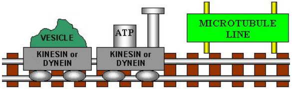
June 2, 2005

Outline

What are Molecular Motors?

Protein molecules in the cell that:

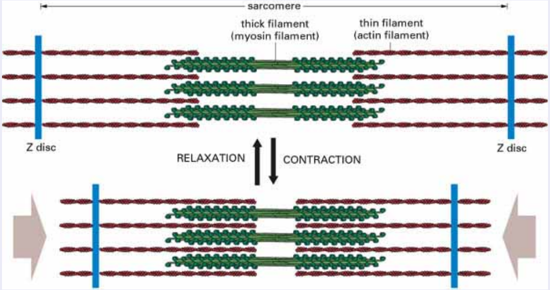
- generate force
- cause transport



Conventional Molecular Motors

Myosin

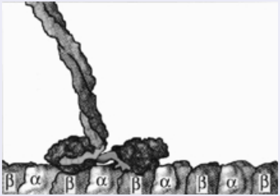
Muscle Contraction



Conventional Molecular Motors

Kinesin

Intracellular Transport

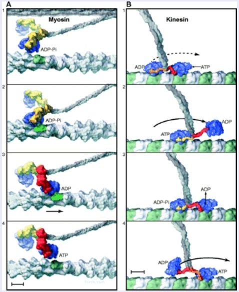


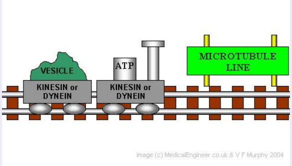
Conventional Molecular Motors

Conventional Molecular Motors

move along polymer tracks

- myosin - actin microfilaments
- kinesin - tubulin microtubules

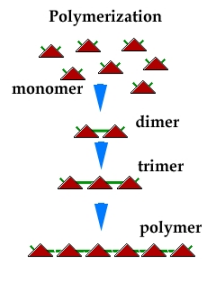




Polymerization as a Motor

Another way to cause motion/transport

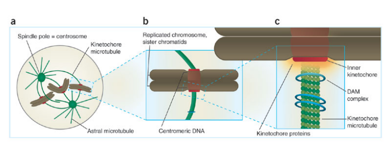
- POLYMERIZATION-or-DEPOLYMERIZATION !
- (adding or subtracting monomers)

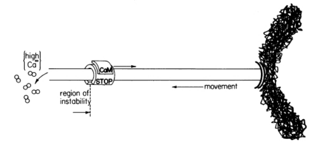


Polymerization as a Motor - Biological Examples

Chromosome Transport During Anaphase

Depolymerization of Spindle Pulls Sister Chromatids Apart:

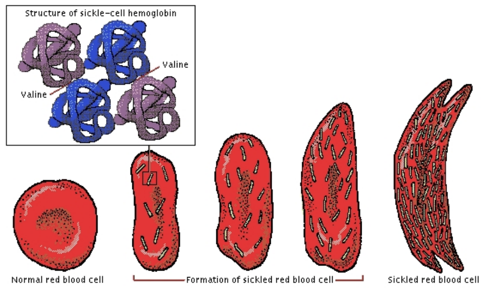


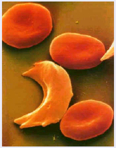


Polymerization as a Motor - Biological Examples

Cell Membrane Deformation

Sickle Hemoglobin Polymerization creates Sickle Cells:





Polymerization as a Motor

How does Polymerization Work?

Rate Constants:

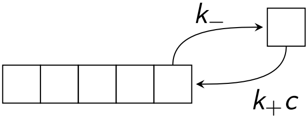
k_+: second order rate constant of adding a monomer

k_-: first order rate constant of subtracting a monomer

c: concentration of monomers in surrounding solution

Note:

Adding/Subtracting monomers may actually require ATP hydrolysis, but this will not be included in our model.



Outline

Polymerization as a Random Walk - Discrete Time

Random Walk Model

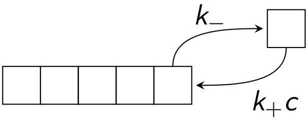
Δx - width of each monomer

Δt - size of discrete time step

$l(t)$ - length of the polymer

$l(0) = m\Delta x$ - inital polymer has m monomers

If $l(t)$ reaches zero, then the polymer is gone, and can no longer grow or shrink.



Polymerization as a Random Walk - Discrete Time

Random Walk Model

At each time step either:

- Add one monomer with probability $k_+ c \Delta t$
- Subtract one monomer with probability $k_- \Delta t$

Then $l(t + \Delta t) = l(t) \pm \Delta x$.

Note:

Let $\Delta t = \frac{1}{k_- + k_+ c}$ so that the total probability at each time step is one:

$$P(-) + P(+) = \frac{k_-}{k_- + k_+ c} + \frac{k_+ c}{k_- + k_+ c} = \frac{k_- + k_+ c}{k_- + k_+ c} = 1$$

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Random Walk - Discrete Time Simulation

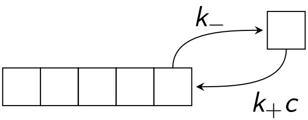
Simulation Procedure

Let $num_- = k_- \Delta t$

At each time step, generate u, a uniform(0,1) random number:

Table: Algorithm for deciding which event occurs.

Condition	Action
$0 \leq u < num_-$	subtract a monomer
$num_- \leq u \leq 1$	add a monomer



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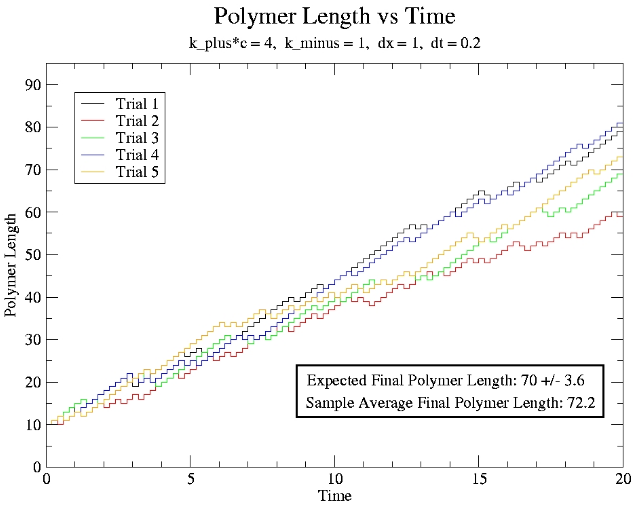
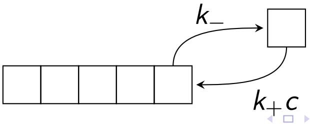


Polymerization as a Random Walk - Continuous Time

Random Walk Model with Continuous Time

- Discrete Time Model is not very realistic. Assume that:
  1. Adding or Subtracting events are independent
  2. In a small amount of time dt:
     - $P_{\text{one event}}(dt) = \lambda dt + o(dt)$
     - $P_{\text{no events}}(dt) = 1 - \lambda dt + o(dt)$
- Number of Events in time t is modeled as a Poisson Process!
  - Rate: $\lambda = k_- + k_+ c$
- Δt is now random
  - Inter-arrival times have exponential(rate=λ) distribution



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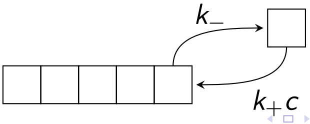

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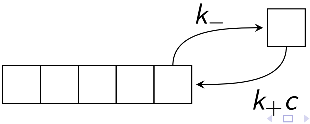


Continuous Time Simulation

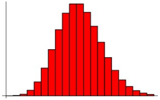
Poisson Process

- Has density function

$$P\left(N(t)=k\right)=\frac{(\lambda t)^k}{k!}e^{-\lambda t}$$

- Often used to describe the number of events that occur in an amount of time t.
- Time between events, τ, given by exponential(rate=λ):

$$P\left(\tau=t\right)=\lambda e^{-\lambda t}$$



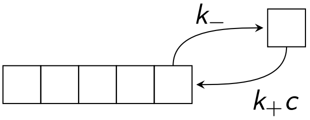
Random Walk - Continuous Time Simulation

Generation of an Exponential from a Uniform

Let U be a uniform(0,1) random variable, and $\frac{1}{\lambda} > 0$, then

$$X = -\frac{1}{\lambda} \log U$$

is an exponential(rate=λ) random variable



Random Walk - Continuous Time Simulation

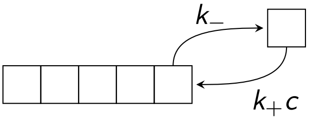
Simulation Set-up

Let the following formulas hold:

- $P(-) = \frac{k_-}{k_- + k_+ c} = \frac{k_-}{\lambda}$
- $P(+) = \frac{k_+ c}{k_- + k_+ c} = \frac{k_+ c}{\lambda}$
- $num_- = \frac{k_-}{\lambda}$

Note that the total probability is still one:

$$P(-) + P(+) = \frac{k_-}{\lambda} + \frac{k_+ c}{\lambda} = \frac{k_- + k_+ c}{k_- + k_+ c} = 1$$



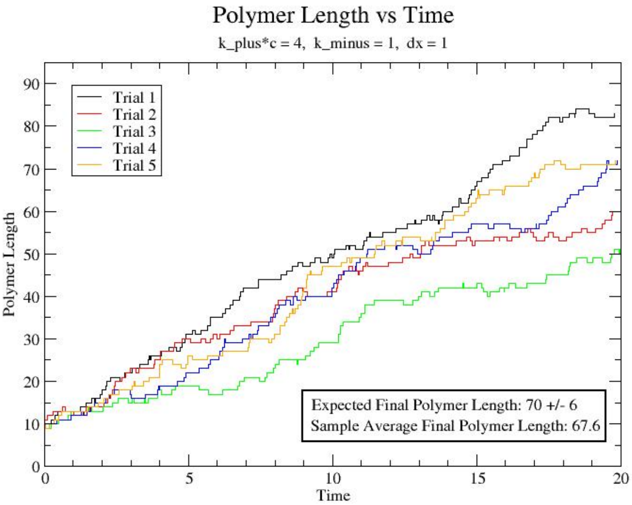
Random Walk - Continuous Time Simulation

Simulation Procedure

For each event-time pair:

1. Generate two uniform(0,1) random numbers, u_1, u_2.
2. Use u_1 to generate the interarrival time, τ, for the event using $\tau = -\frac{1}{\lambda} \log u_1$.
3. Use u_2 to decide whether the event will be addition or subtraction:
   - If $0 \leq u_2 < num_-$ then subtract a monomer.
   - If $num_- \leq u_2 \leq 1$ then add a monomer.
4. Record the i^{th} event time $t_i = t_{i-1} + \tau$ and the location of the end of the polymer $x_i = x_{i-1} \pm \Delta x$, where $\pm$ is determined by Step 3.

Random Walk - Continuous Time Simulation

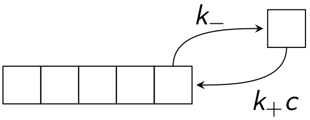


Brownian Motion

Random Walk - Brownian Motion Connection

Let $\alpha = k_+ c$, $\beta = k_-$.
$p(x,t)$:probability that the polymer has length x at time t (continuous time)

- $p_t(x,t) = \alpha p(x-\Delta x, t) + \beta p(x+\Delta x, t) - (\alpha+\beta) p(x,t)$



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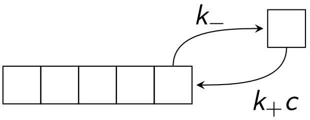

Brownian Motion

Random Walk - Brownian Motion Connection

- Taylor Expansion & Some Algebra:

$$\begin{aligned} p_t(x,t) &= (\alpha+\beta)\frac{(\Delta x)^2}{2} p_{xx}(x,t) \\ &- (\alpha-\beta)\Delta x \; p_x(x,t) \\ &+ \text{higher order terms in } \Delta x \end{aligned}$$

- Let $\Delta x \to 0$:

$$\lim_{\Delta x \to 0} (\alpha+\beta)\frac{(\Delta x)^2}{2} = D \qquad \lim_{\Delta x \to 0} (\alpha-\beta)\Delta x = V$$

Brownian Motion

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Brownian Motion

Random Walk - Brownian Motion Connection

- Then we obtain

$$p_t(x,t) = Dp_{xx}(x,t) - Vp_x(x,t)$$

- The Diffusion Equation with Drift!
- Will allow us to answer more questions later...

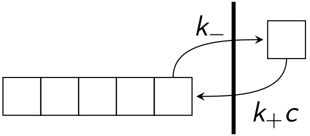
Outline

Continuous Time Simulation with a Fixed Wall

Polymer Interacting with a Fixed Wall

Let $x = w$ be the position of the fixed wall.
Polymer (and Simulation) behaves as before, but with additional constraints:

- If $w - x < \Delta x$ then a monomer cannot be added.
- If a monomer is to be added and $w - x < \Delta x$, then polymer length remains the same at that time.



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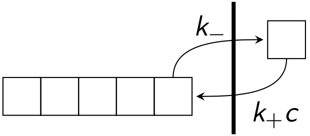

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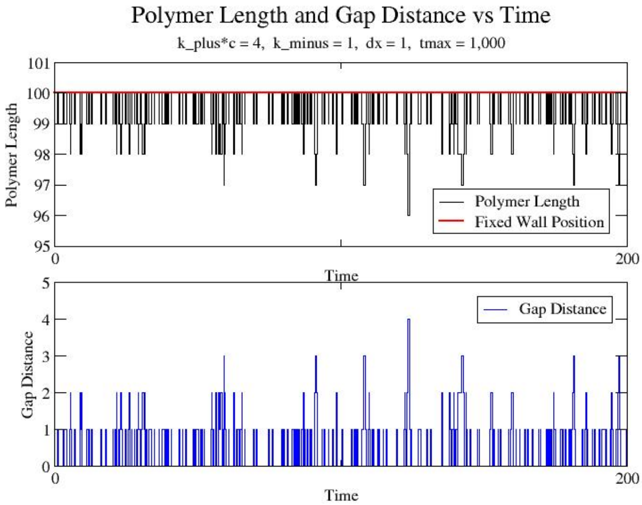


Continuous Time Simulation with a Fixed Wall

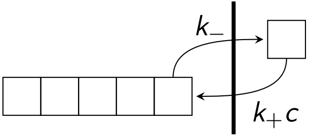
Gap Distribution

We can also model the gap distance using the diffusion equation with drift:

- $p_t = Dp_{xx} + Vp_x$

$$D = (k_+ c + k_-) \qquad V = (k_+ c - k_-)$$

- Note that the sign on V is different than before.
- We can solve for the steady state solution



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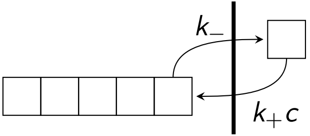

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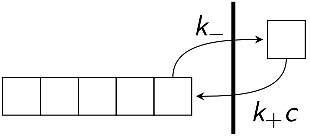

Continuous Time Simulation with a Fixed Wall

Steady State Gap Distribution - Brownian Motion

$0 = Du_{xx} + Vu_x$

Need two conditions:

- No-Flux Boundary Condition at x=0:

$$Du_x + Vu = 0$$

- Normalization:

$$\int_0^\infty u(x)dx = 1$$

- Steady-State Solution:

$$u(x) = \frac{V}{D}e^{-\frac{V}{D}x}$$

- Note: This model is spatially continuous system...

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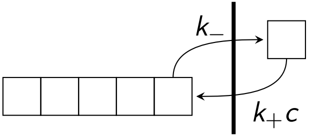

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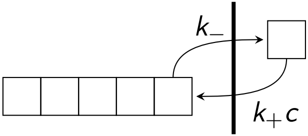

Continuous Time Simulation with a Fixed Wall

Steady State Gap Distribution - Random Walk

Let $p_i = \mu^i$:

- $\mu = \alpha\mu^2 + \beta$
- Quadratic Equation & $\alpha + \beta = 1$:

$$\mu_1 = 1, \qquad \mu_2 = \frac{\beta}{\alpha}$$

- Then we know that the system must be of the form

$$p_i = a\left(\frac{\beta}{\alpha}\right)^i + b$$

Continuous Time Simulation with a Fixed Wall

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Continuous Time Simulation with a Fixed Wall

Steady State Gap Distribution - Random Walk

We can apply the normalization condition:

$$\sum_{i=0}^{\infty} p_i = \sum_{i=0}^{\infty} (a \left(\frac{\beta}{\alpha}\right)^i + b) = 1$$

- The sum must converge, so $b = 0$
- We are left with a geometric series:

$$a \sum_{i=0}^{\infty} \left(\frac{\beta}{\alpha}\right)^i = a \frac{1}{1 - \frac{\beta}{\alpha}} = 1$$

- Spatially Discrete Steady State Solution:

$$p_i = \frac{\alpha - \beta}{\alpha} \left(\frac{\beta}{\alpha}\right)^i$$

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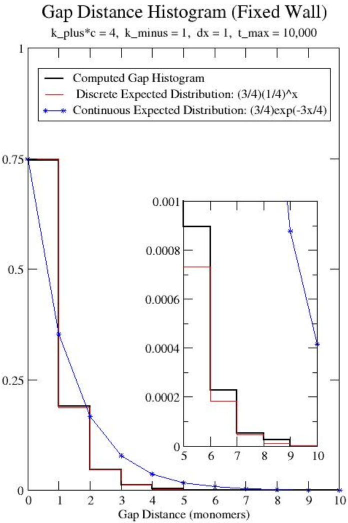
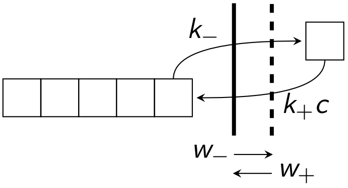


Simulation Including a Moving Wall

Wall Moves According to a Random Walk

w_+ - rate that the wall moves towards the polymer
w_- - rate the wall moves away from the polymer

g - gap distance
$\lambda_p = k_+ c + k_-$ - Poisson Process rate for the polymer
$\lambda_w = w_+ + w_-$ - Poisson Process rate for the wall

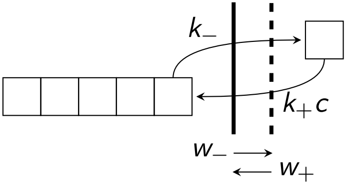


Simulation Including a Moving Wall

Polymer Interacting with a Moving Wall

Polymer and Wall both follow random walks with constraints:

- If $g < \Delta x$ then a monomer cannot be added and the wall cannot move towards the polymer.
- If a monomer is to be added (wall is to move towards the polymer) and $g < \Delta x$, then polymer length (wall position) remains the same at that time.



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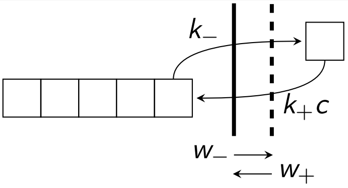

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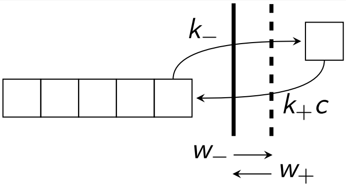

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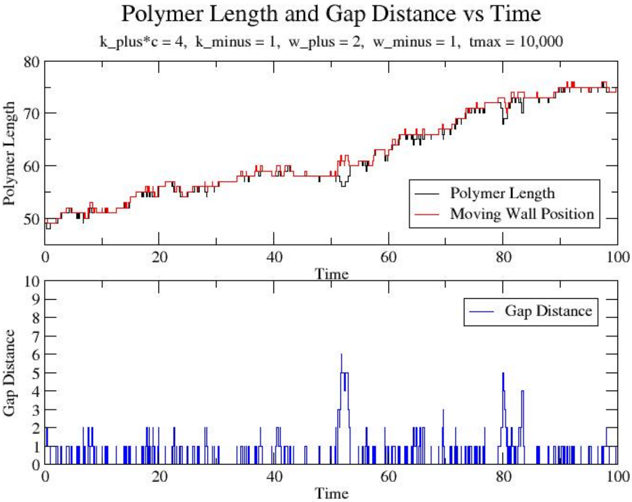


Simulation Including a Moving Wall

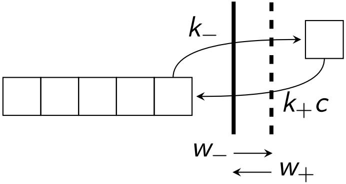
Steady State Gap Distribution - Random Walk

Let p_i denote the probability that the gap distance is i, and let

$$\alpha_p = \frac{k_+ c}{k_+ c + k_- + w_+ w_-} \qquad \beta_p = \frac{k_-}{k_+ c + k_- + w_+ w_-}$$
$$\alpha_w = \frac{w_+}{k_+ c + k_- + w_+ w_-} \qquad \beta_w = \frac{w_-}{k_+ c + k_- + w_+ w_-}$$

- $p_i = (\alpha_p + \alpha_w) p_{i+1} + (\beta_p + \beta_w) p_{i-1}$

(There are now 2 ways that gap distance can change)



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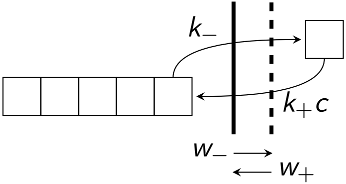


Simulation Including a Moving Wall

Steady State Gap Distribution - Random Walk

Let $\alpha = \alpha_p + \alpha_w$, and $\beta = \beta_p + \beta_w$

Then we can see that

$$
\begin{aligned}
p_i &= (\alpha_p + \alpha_w) p_{i+1} + (\beta_p + \beta_w) p_{i-1} \\
&= \alpha p_{i+1} + \beta p_{i-1}
\end{aligned}
$$

This is exactly the same equation we had before!

Simulation Including a Moving Wall

Steady State Gap Distribution - Random Walk

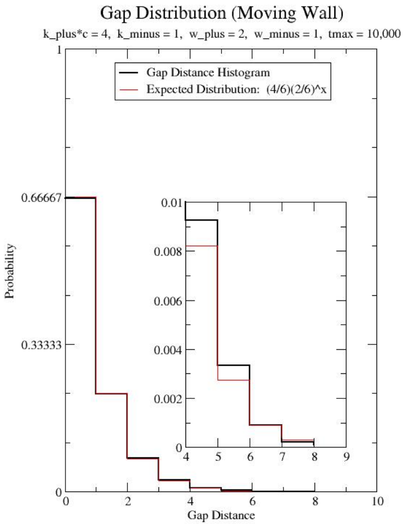
We already know the Steady State Distribution:

$$p_i = \frac{\alpha - \beta}{\alpha} \left(\frac{\beta}{\alpha} \right)^i$$

where:

$$\alpha = (k_+ c + w_+) \qquad \beta = (k_- + w_-)$$

Simulation Including a Moving Wall



Simulation with many Polymers

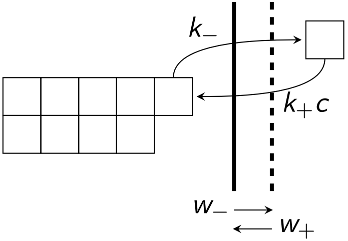
Multiple Polymers Interacting with a Moving Wall

w_+ - rate that the wall moves towards the polymers

w_- - rate the wall moves away from the polymers

$\lambda_p = k_+c + k_-$ - Poisson Process rate for each polymer

$\lambda_w = w_+ + w_-$ - Poisson Process rate for the wall



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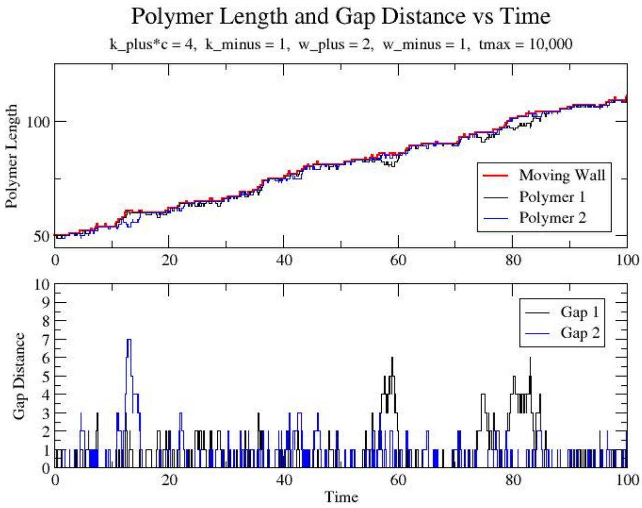
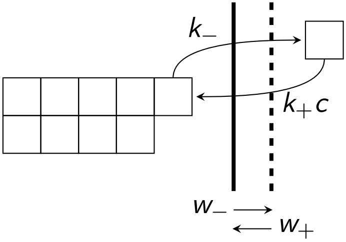


Simulation with many Polymers

Multiple Polymers Interacting with a Moving Wall

- The Polymers are *Identical*:
  - $k_+ c_{p1} = k_+ c_{p2} = k_+ c$
  - $k_{-\,p1} = k_{-\,p2} = k_-$
- Are the Polymers *Independent*?



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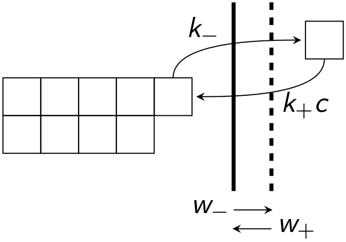

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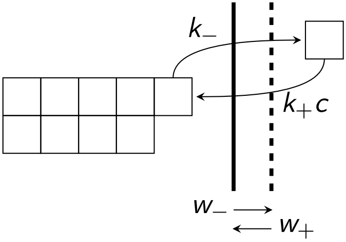


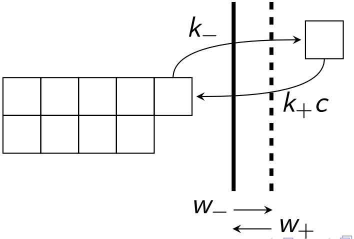
Simulation with many Polymers

Multiple Polymers Interacting with a Moving Wall

If the Polymers are *Independent*:

- Steady State Distribution for each Polymer should be the same as in the Single-Polymer Case:

$$p_{1_i} = p_{2_i} = \frac{\alpha - \beta}{\alpha} \left(\frac{\beta}{\alpha} \right)^i$$



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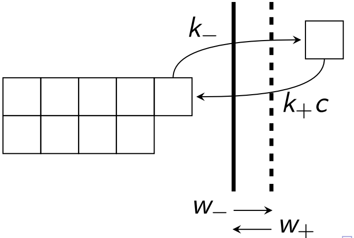
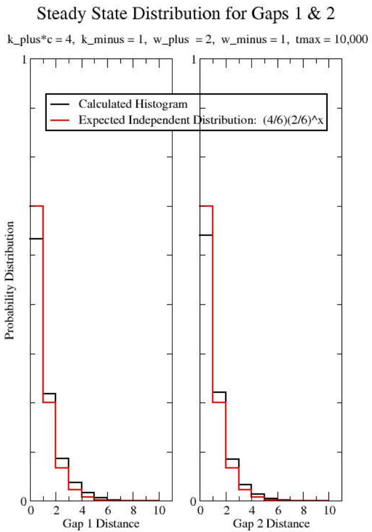


Simulation with many Polymers



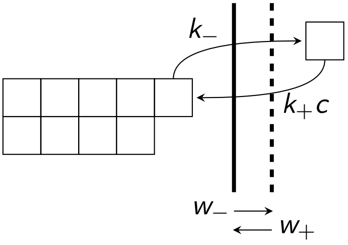
Simulation with many Polymers

Polymer Cooperation

Polymers are not Independent ⇒ Cooperation!

How? (Mathematically)

- Look at the Polymers from the Point of View of the Wall.



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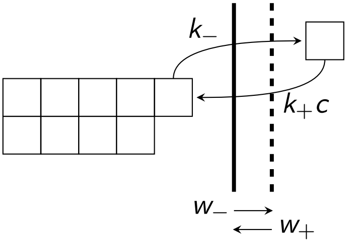


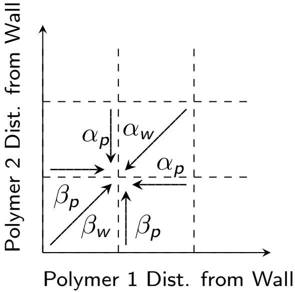
Polymer Cooperation - 2D Random Walk

Polymer Motion from Wall's POV - Gap Distances

Rates of motion are given by:

polymer moves	wall moves
α_p - towards wall	α_w - towards polymer
β_p - away from wall	β_w - away from polymer

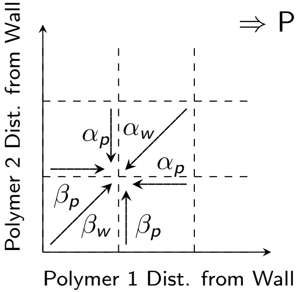
(Origin represents both polymers touching the wall)



Polymer Cooperation - 2D Random Walk

$p(x, y, t)$ - gap 1 distance is x , gap 2 distance is y, at time t

$$
\begin{aligned}
p_t(x,y,t) &= \alpha_p\left(p(x+\Delta x, y, t) + p(x, y+\Delta y, t)\right) \\
&+ \beta_p\left(p(x-\Delta x, y, t) + p(x, y-\Delta y, t)\right) \\
&+ \alpha_w\ p(x+\Delta x, y+\Delta y, t) \\
&+ \beta_w\ p(x-\Delta x, y-\Delta y, t) \\
&- (2\alpha_p + 2\beta_p + \alpha_w + \beta_w)\, p(x,y,t)
\end{aligned}
$$



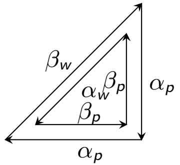
$\Rightarrow$ PDE...

Polymer Cooperation - Another View

Smallest Cycle

Net Motion	Physical Result	Condition
Clockwise	polymer pushes wall	$\gamma > 1$
Counterclockwise	wall pushes polymer	$\gamma < 1$
None	balance	$\gamma = 1$

$$\gamma = \frac{\beta_w {\alpha_p}^2}{\alpha_w {\beta_p}^2}$$

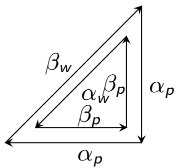


Polymer Cooperation - Another View

Smallest Cycle

$$\log\gamma = \log\frac{\beta_w{\alpha_p}^2}{\alpha_w{\beta_p}^2} = \log\left(\frac{\alpha_p}{\beta_p}\right)^2 - \log\frac{\alpha_w}{\beta_w}$$

$$= 2\log\frac{\alpha_p}{\beta_p} - \log\frac{\alpha_w}{\beta_w}$$



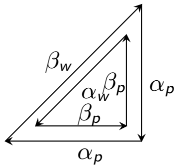
Polymer Cooperation - Another View

Smallest Cycle - Force Connection

Net Motion	Physical Result	Condition
Clockwise	polymer pushes wall	$\log\gamma > 0$
Counterclockwise	wall pushes polymer	$\log\gamma < 0$
None	balance	$\log\gamma = 0$

$$\frac{k_B T}{\Delta x}\log\gamma = \frac{k_B T}{\Delta x}\left(2\log\frac{\alpha_p}{\beta_p} - \log\frac{\alpha_w}{\beta_w}\right)$$

$$\text{Net Force} = \text{Force of 2 Polymers} - \text{Force of Wall}$$



The End

Questions?