Stochastic Cells \*

Dimerization: monomer (*M*) joins up with another monomer and becomes a dimer (*D*): 2*M* ↔ *D*. The forward reaction rate is and the backward reaction rate is . There are two reactions:

* the backward unbinding reaction () rate per unit volume is ,
* the forward binding reaction rate () per unit volume is . Assume that: = 1n, = 2 , at *t* = 0 are only *N* monomers.

1. Continuum dimerization. Find equations for d*M*/d*t,* d*D*/d*t* and write code to simulate continuum dimerization.
2. Stochastic dimerization. Implement algorithm:
3. Calculate a list of the rates of all reactions in the system.

for discrete molecules:

,

,

1. Find the total rate (*):*
2. Pick a random time with probability distribution: .
3. If the current time *t* is bigger than , no further reactions will take place, end.
4. Otherwise:

* increment *t* by ,
* pick a random number *r* uniformly distributed in the range [0, ),
* pick the reaction j:

if *r* < :2*M* → *D*

else: *D* → 2*M,*

* execute that reaction by incrementing each chemical involved by its stoichiometry

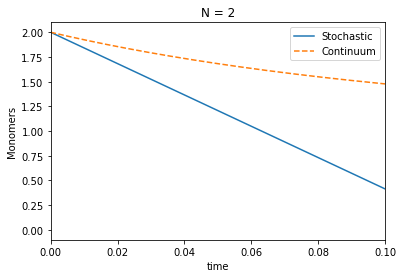
1. Repeat.

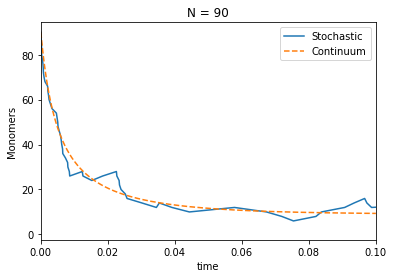
**C)** Compare A) and B) for:

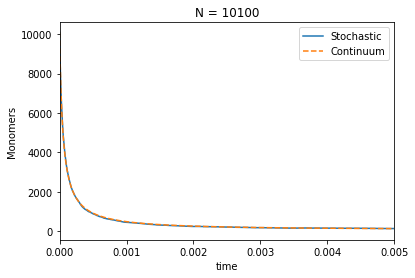
*N* = 2, *N* = 90 and *N* = 10 100.

**\*** The assignment is from the book “Statistical Mechanics: Entropy, Order, Parameters and Complexity” by James Sethna (p. 178-179).

Results:







Hints:

**A)**

equations for: d*M*/d*t* and d*D*/d*t*:

to calculate the integrate you can use: scipy.integrate.odeint()

**B)**

to find use scipy.stats.expon.rvs(), remember to set scale,

to choose *r* use random.randrange().