

May 9, 2012

Instructions for simulating a polymer size distribution with XPP.

NOTE: it is likely that Matlab would be easier for this task, but we can do it with XPP if we do not have a convenient way to run Matlab.

The following file can be used for simulating a polymer size distribution from size 0 (monomers) to size 100. Here the first step requires dimerization, and every following step is single monomer addition.

Ode file:

```
# asizedis.ode
# polymer size distribution
# simple polymerization
# Mar 4, 2006

# xj= number of fibers of length j
# a= conc of monomers
# kf, kr = forward and reverse rate constants

par kf=10, kr=1, kinit=0.005, adepl=1
a(0)=20
sm99=x100
sm[98..2]=sm[j+1]+x[j+1]

#eqn for monomers:
# Set adepl=1 for constant total amt, 0 for fixed monomer level
a' = adepl*(-kf*a*(sm2-x100+x2)+kr*(sm2+x2))

# initialization from dimers
x1'= kinit*a*a+kr*x2-kf*a*x1
x[2..99]'= kf*a*(x[j-1]-x[j])+kr*(x[j+1]-x[j])
x100' = -kr*x100+kf*a*x99

#Computing the total number of fibers
Nf=sm2+x2+x1
aux Ntotal=Nf

# computing the total and mean length of fibers
p1=sum(2,100)of(i'*shift(x2,i'-2))+x1
aux Ltotal=p1
aux Lmean=p1/(Nf+1e-8)
@ bounds=10000000, meth=gear, dt=0.05, total=100
done
```

Fire up an XPP window and integrate this file  
Initial conditions Go (I G)

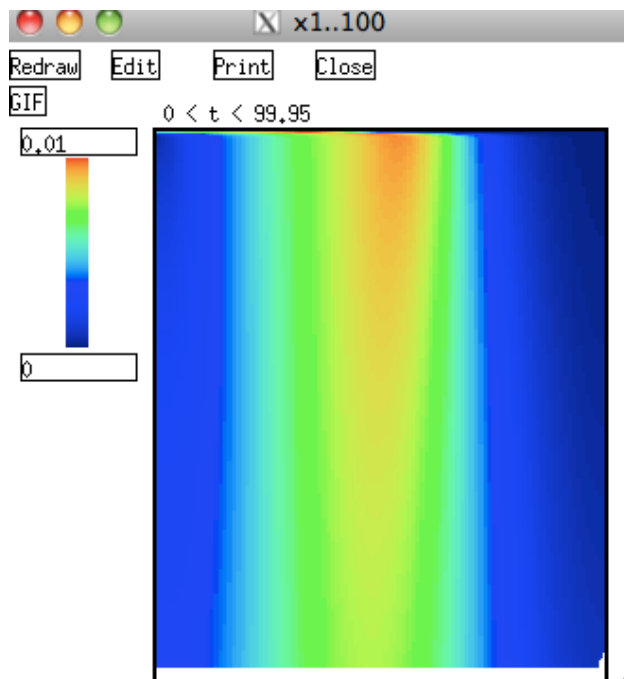
To plot results in array form select

Viewaxes Array

Then fill in the table as follows:

Click OK. A window will come up. You may need to click "Redraw" in that window.

You will get a color plot that looks like this:



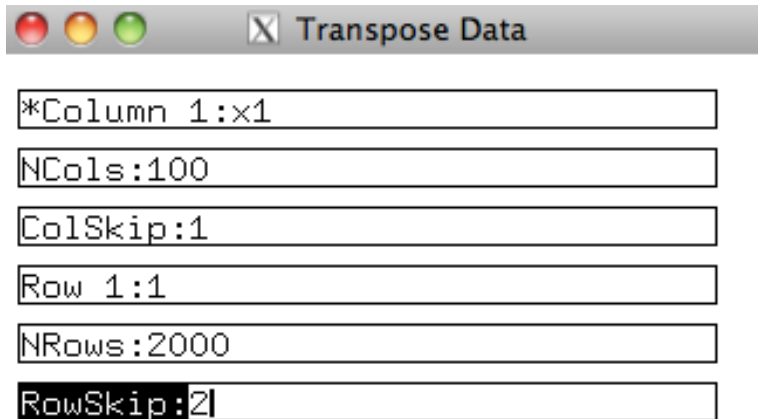
| Edit arrayplot |      |
|----------------|------|
| *Column 1:     | x1   |
| NCols:         | 100  |
| Row 1:         | 0    |
| NRows:         | 2000 |
| RowSkip:       | 1    |
| Zmin:          | 0    |
| Zmax:          | 0.01 |
| Autoplot(0/1): | 0    |
| ColSkip:       | 1    |

The data has 100 columns of polymer sizes (x1.. x100) and 2000 rows of time points based on our choice of  $\Delta t=0.05$ , Total time =100.

We can also create a set of line plots for the distribution versus time using the Transpose option.

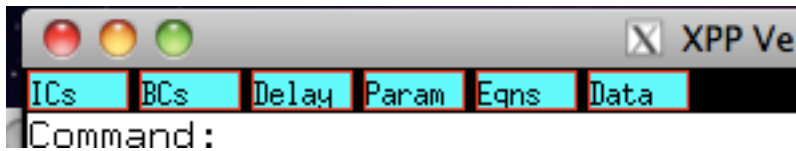
File Transpose (F T)

Fill in the table as follows to see the early time behaviour:

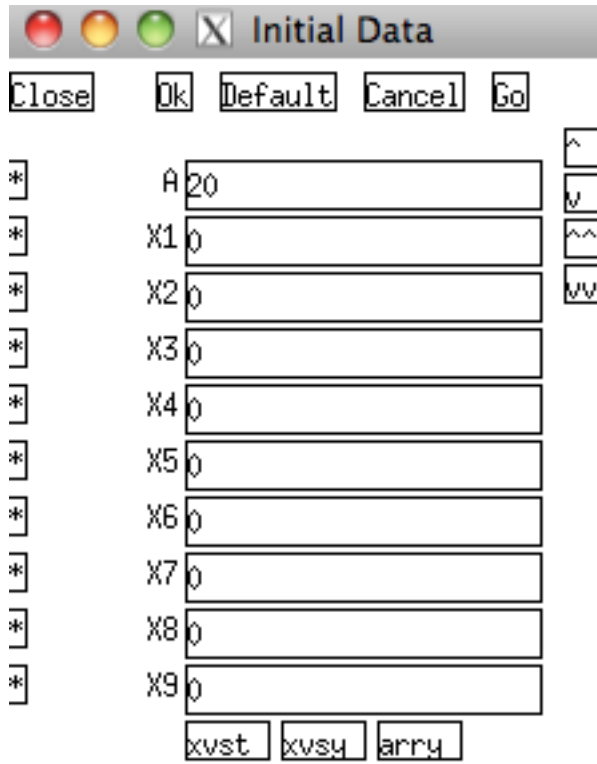


HERE IS A HANDY WAY TO PLOT A BUNCH OF CURVES AND HAVE THEM ALL SAVED SO YOU CAN MAKE A NICE PLOT WITH MANY PROFILES.

Now select the IC's button on

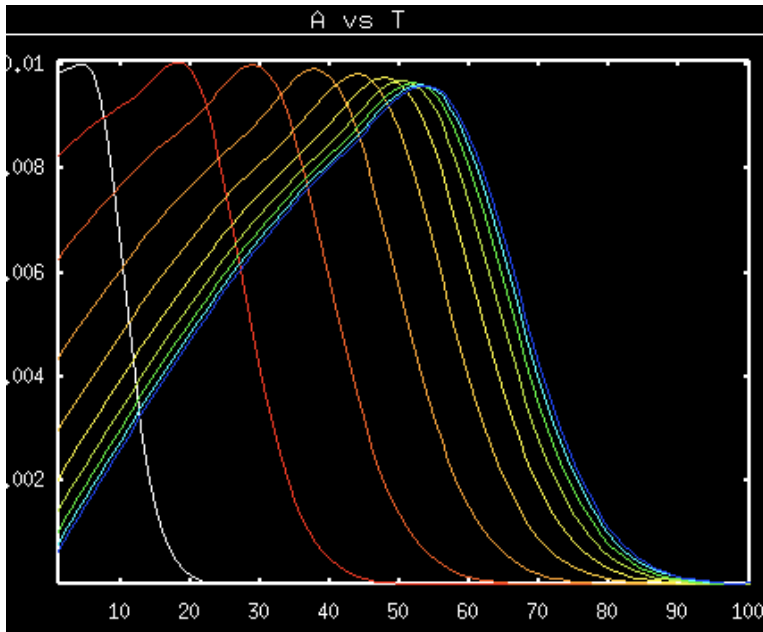


Check each of the boxes on the left to get

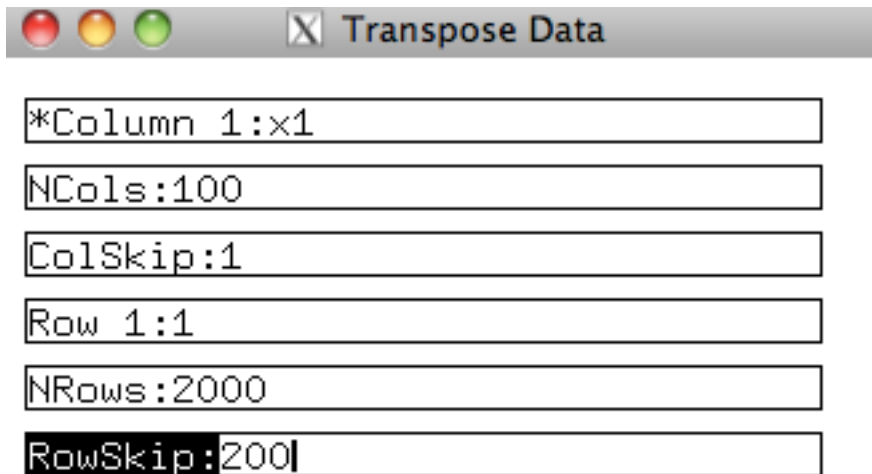


Then click on the xvst at the bottom of this little window.

You will see this plot appear:



If we want to see later time behaviour we can repeat the simulation with the same steps but at the Transpose panel we fill in



This skips more rows (= time steps) between plots.

We then get:

