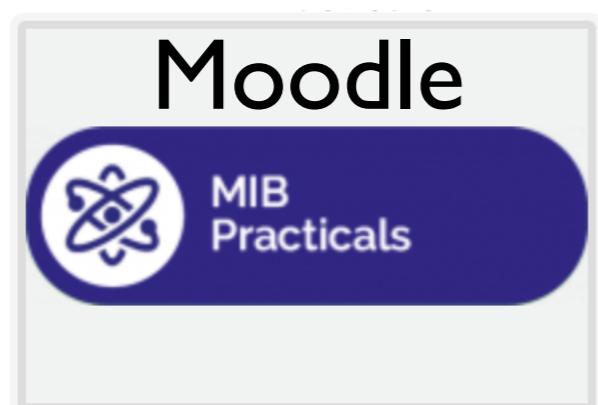
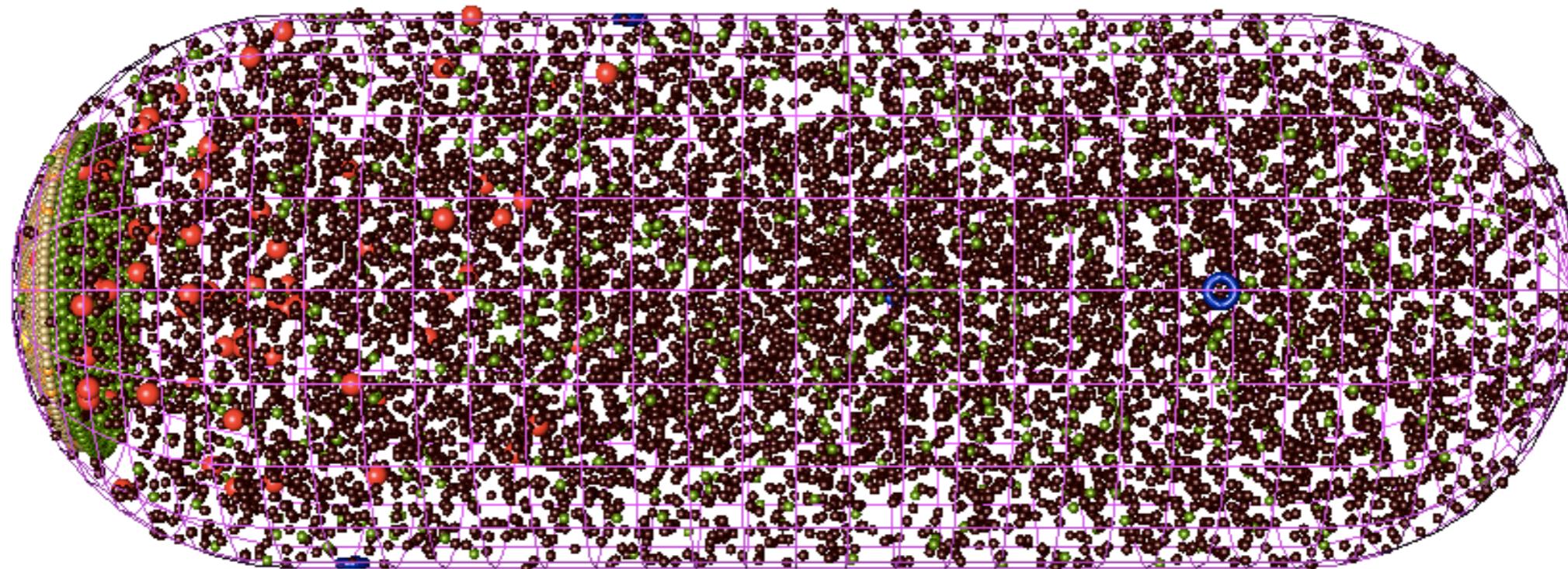


Karen Lipkow

# Smoldyn I



MIB2 practical slides&scripts:  
MIB2.2\_stages: these slides  
MIB2.2\_script: lesson script

# Summary MIB2.2

How to run Smoldyn

Introduction to the chemotaxis system of *Escherichia coli*

Build a Smoldyn model of the *E. coli* chemotaxis system

# Summary of Smoldyn workflow

## Text configuration file

```
# Simulation file for Lotka-Volterra reaction

graphics opengl
graphic_iter 5

dim 2
species rabbit fox
# max_mol 20000

boundaries 0 -100 100 p
boundaries 1 -100 100 p

time_start 0
time_stop 20
time_step 0.001

color rabbit 1 0 0
color fox 0 1 0
display_size rabbit 2
display_size fox 3

molecule_lists rlist plist
mol_list rabbit rlist
mol_list fox plist
molperbox 1

difc all 100
reaction r1 rabbit -> rabbit + rabbit 10
reaction r2 rabbit + fox -> fox + fox 8000
reaction r3 fox -> 0 10

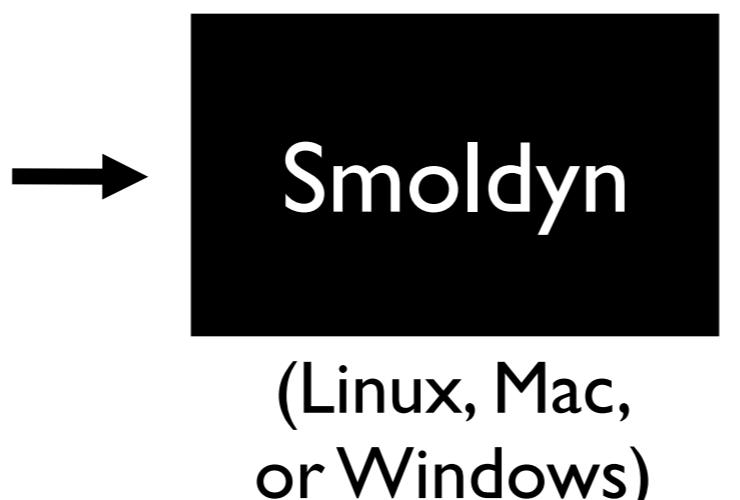
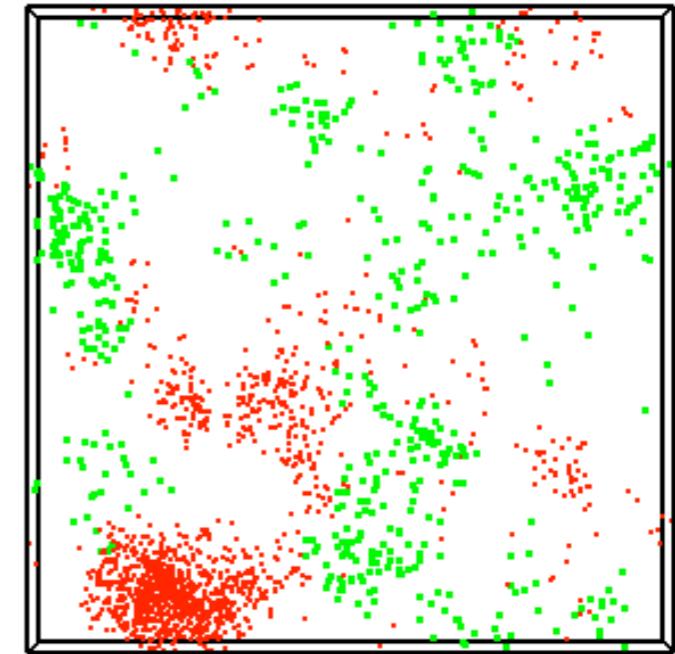
mol 1000 rabbit u u
mol 1000 fox u u

output_files lotvoltout.txt
cmd i 0 5 0.01 molcount lotvoltout.txt

end_file
```

make into movies:  
GraphicConverter,  
QuickTime, ...

## Real-time graphics

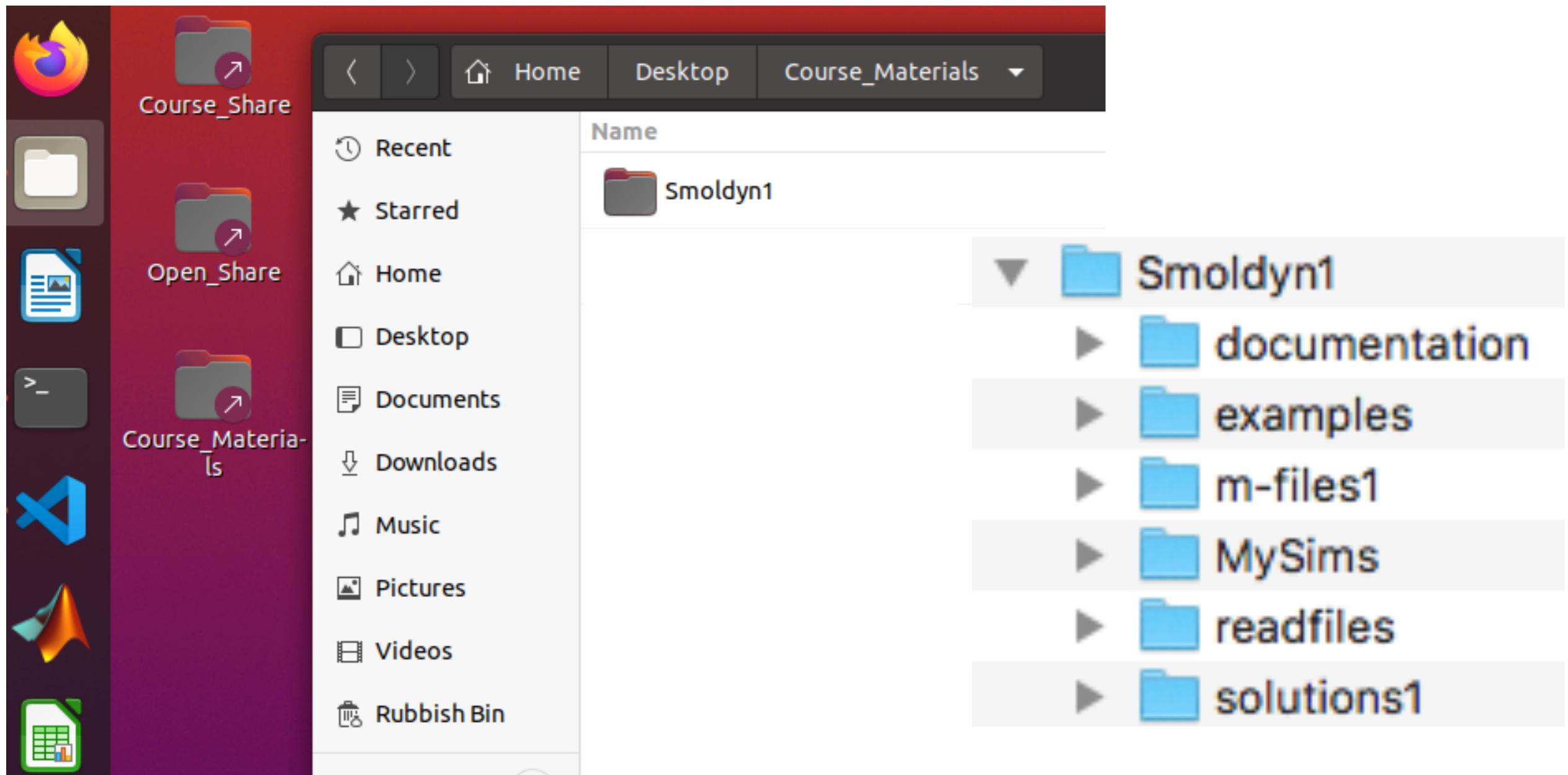


analyse, plot:  
MATLAB, R, ...

## Text output

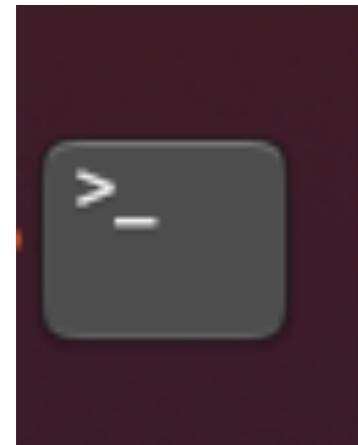
0.02 24 0 1 76 0 0 100 0	0 0 100 0	0 0 100 0
1.02 25 0 2 75 0 0 100 0	0 0 100 0	0 0 100 0
2.02 25 0 2 75 0 0 100 0	0 0 100 0	0 0 100 0
3.02 26 0 3 74 0 0 100 0	0 0 100 0	0 0 100 0
4.02 26 0 3 74 0 0 100 0	0 0 100 0	0 0 100 0
5.02 26 0 3 74 0 0 100 0	0 0 100 0	0 0 100 0
6.02 26 0 3 74 0 0 100 0	0 0 100 0	0 0 100 0
7.02 26 0 3 74 0 0 100 0	0 0 100 0	0 0 100 0
8.02 25 0 2 75 0 0 100 0	0 0 100 0	0 0 100 0
9.02 24 0 1 76 0 0 100 0	0 0 100 0	0 0 100 0
10.02 25 0 2 75 0 0 100 0	0 0 100 0	0 0 100 0
11.02 25 0 2 75 0 0 100 0	0 0 100 0	0 0 100 0
12.02 26 0 3 74 0 0 100 0	0 0 100 0	0 0 100 0
13.02 27 0 4 73 0 0 100 0	0 0 100 0	0 0 100 0
14.02 27 0 4 73 0 0 100 0	0 0 100 0	0 0 100 0
15.02 28 0 4 72 0 0 100 0	0 0 100 0	0 0 100 0
16.02 28 0 4 72 0 0 100 0	0 0 100 0	0 0 100 0
17.02 30 0 6 70 0 0 100 0	0 0 100 0	0 0 100 0
18.02 30 0 6 70 0 0 100 0	0 0 100 0	0 0 100 0
19.02 31 0 7 69 0 0 100 0	0 0 100 0	0 0 100 0
20.02 31 0 7 69 0 0 100 0	0 0 100 0	0 0 100 0
...		

# Go to Course\_Materials/Smoldyn1



# Use Terminal and Finder to enter Directory of Config files

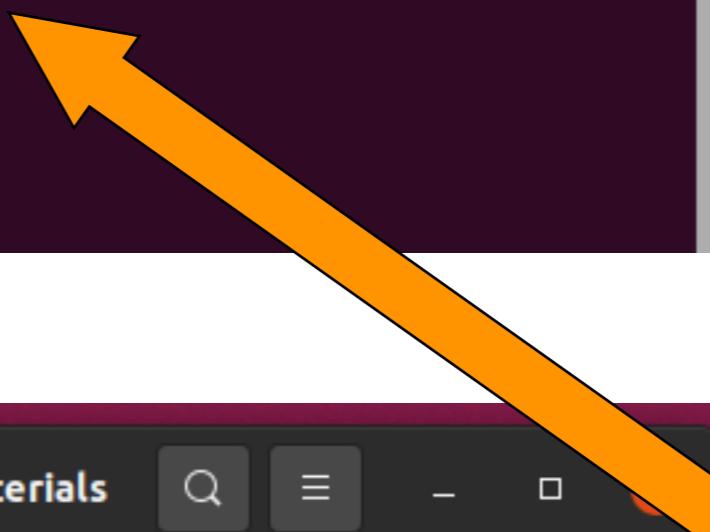
cd Smoldyn1/examples/S8\_reactions/lotvolt



cd <space> dragged folder <enter>

Smoldyn1	
Name	
examples	
S1_intro	
S2_config	
S3_space	
S4_molecules	
S5_graphics	
S6_commands	
S7_surfaces	
S8_reactions	
2Dreact	
allostery	
benchmark	
bireact	
bistable	
bounce	
conf_spread	
equil	
intersurface	
lmbdarho	
lotvolt	Selected
tracking	
unireact	
wallreact	
wildcards	
zeroreact	
S9_compartments	
S10_boxec	

```
participant@brewery: ~/Course_Materials
(base) participant@brewery:~/Course_Materials$ cd
```



```
participant@brewery: ~/Course_Materials
(base) participant@brewery:~/Course_Materials$ cd '/home/participant/Desktop/Cou
rse_Materials/Smoldyn1/examples/S8_reactions/lotvolt'
```

# Basic Unix Commands

**cd = change directory**

type behind “\$”:

```
cd Smoldyn1/examples/S8_reactions/lotvolt
```

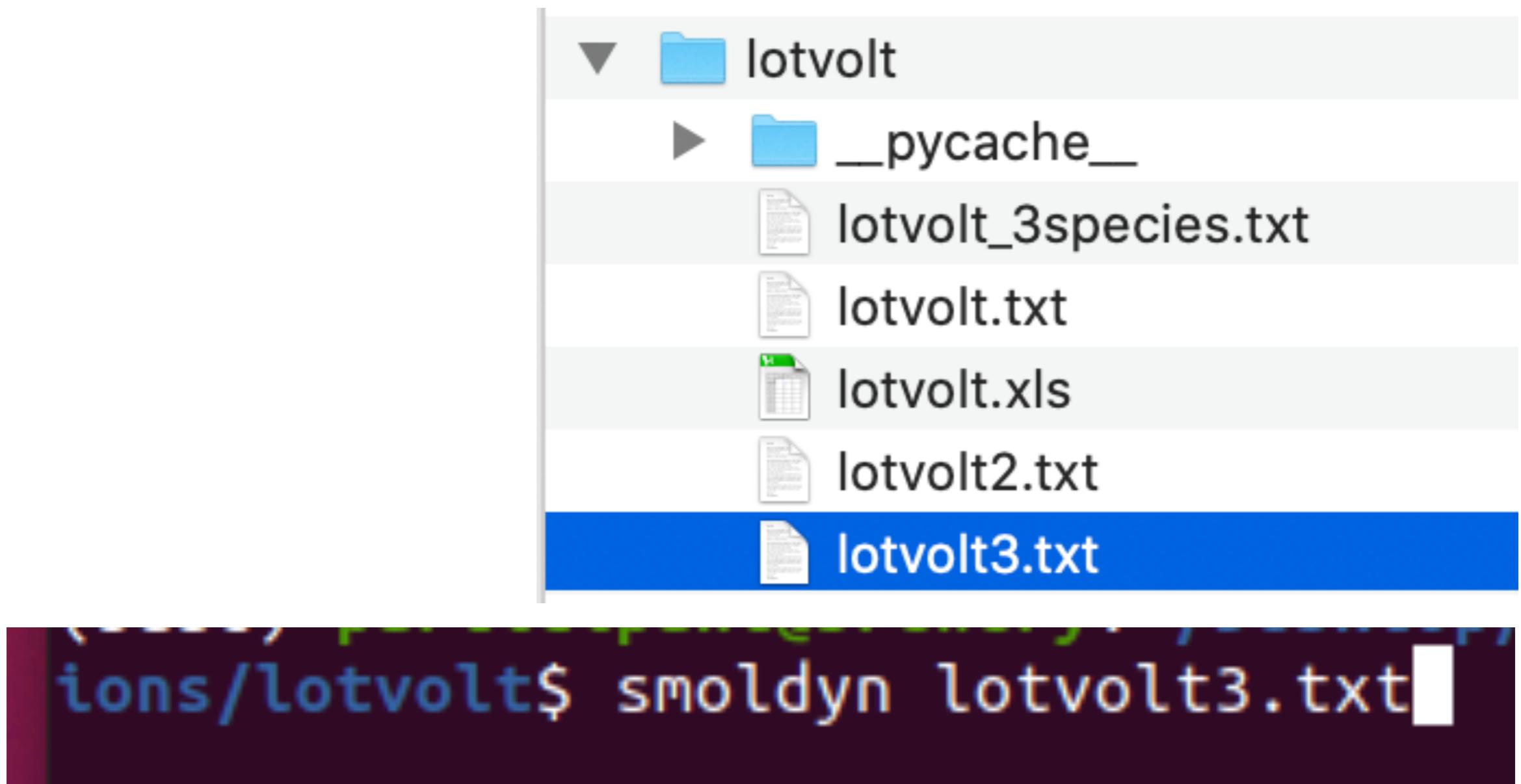
Tab → to complete file name

**cd ..** moves up one level

**ls = list** names of files in the current directory

Thirty Useful Unix Commands in “documentation/MIB2\_docs1” directory

# Start Smoldyn Simulation from Terminal





Open Share



Course\_Materials

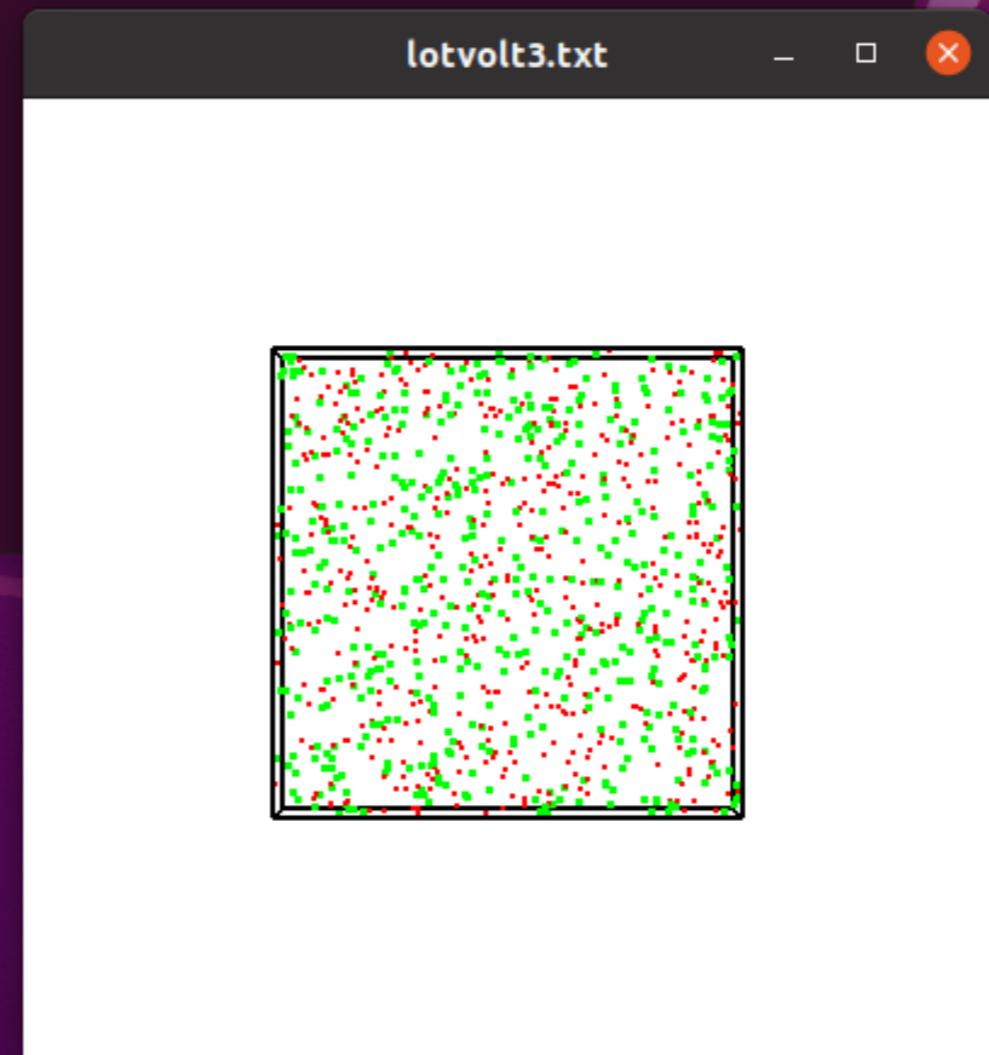
```
participant@brewery: ~/Desktop/Course_Materials/Smoldyn...          -  x
characteristic time: 0.1
conditional reaction probability per time step: 0.00995017

ORDER 2 REACTION PARAMETERS
1 reactions defined
Reactive molecule lists: diffuselist+diffuselist
Reactants, sorted by molecule species:
A+B : r2
Reaction details:
Reaction r2: A + B -> B + B
requested and actual rate constants: 2000, 2000.01
characteristic time: 0.199999
binding radius: 1.16411
unbinding radius: 0

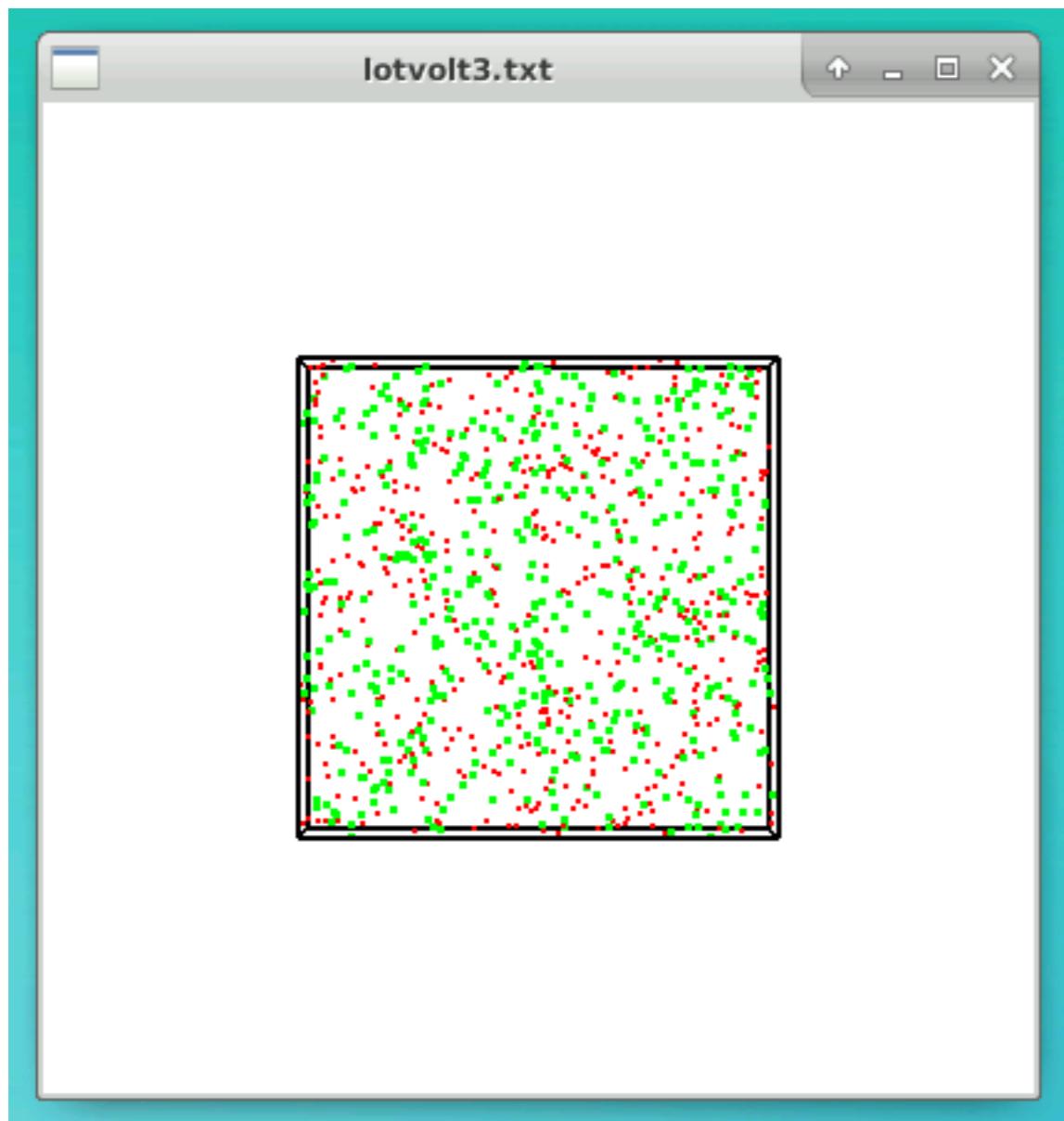
RULES:
none

PARAMETER CHECK
No errors
No warnings

Simulation paused at simulation time: 0
```



# Interactions with the graphics window



To unpause or pause: press  
<space> bar

To stop: click on graphics  
(OpenGL) window, <shift-q>  
(and again to quit)

Zoom out and in by pressing the  
minus <-> and equal <=> keys

Rotate the system using the arrow  
keys and <x>, <y>, <z>

# Common errors and warnings (stdout)

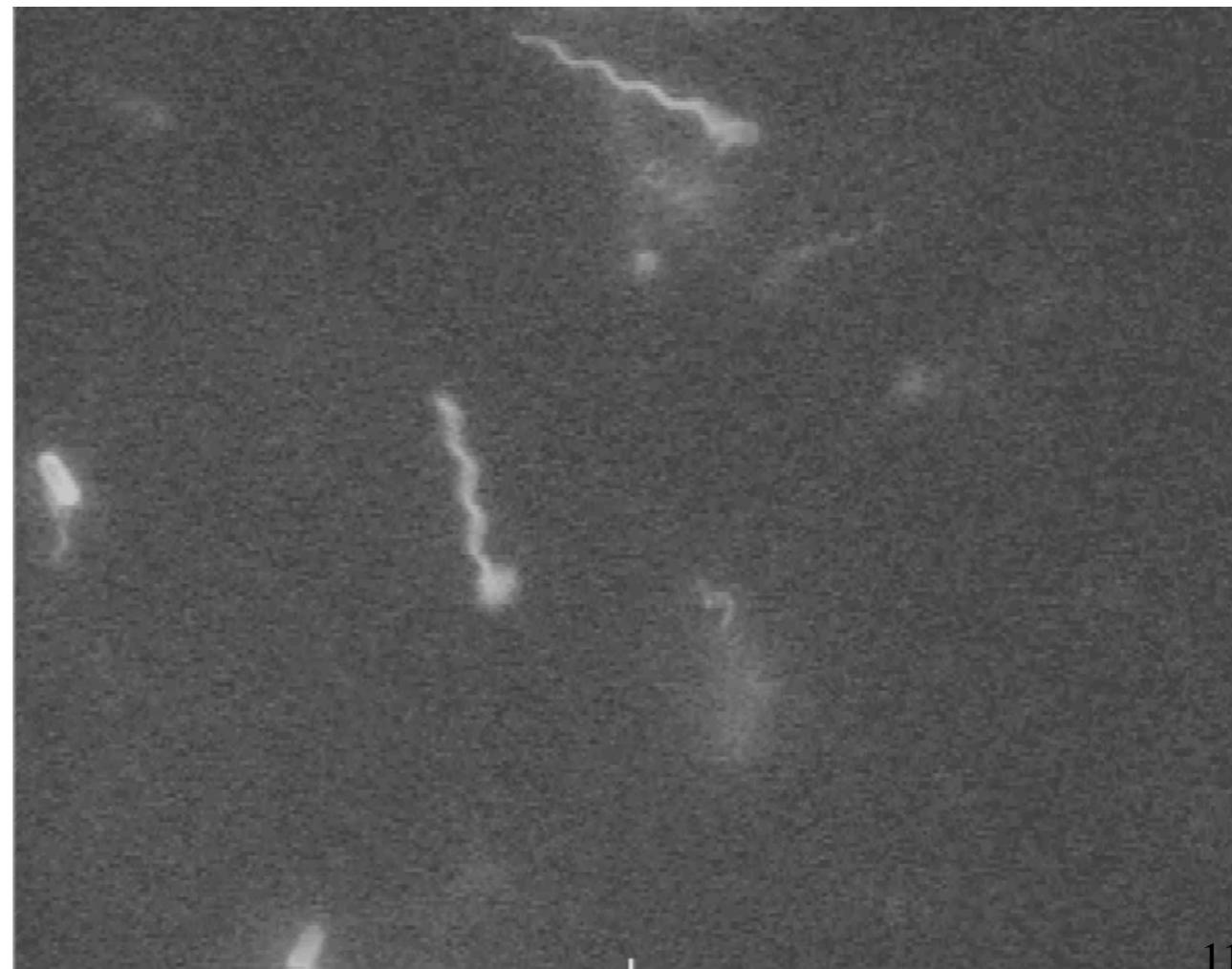
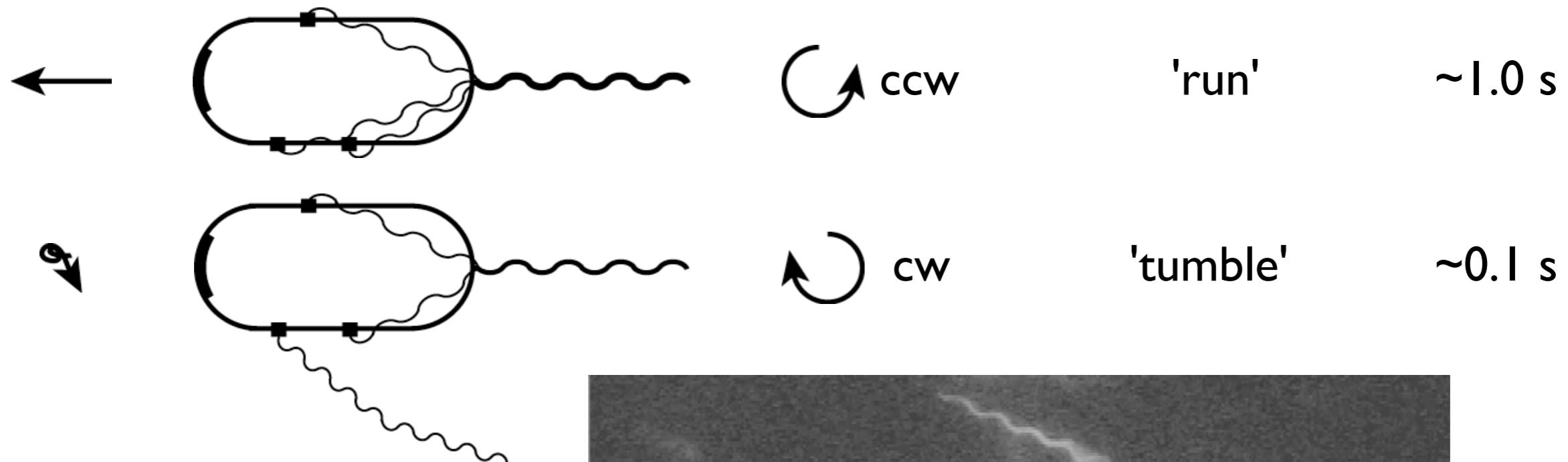
## Errors:

file not found: all files (config file, readfiles) in current directory?  
file not found: exact name of file, incl. extensions (.txt) - not always displayed  
file cannot be read: line endings - Unix, Windows or Mac

## Warnings:

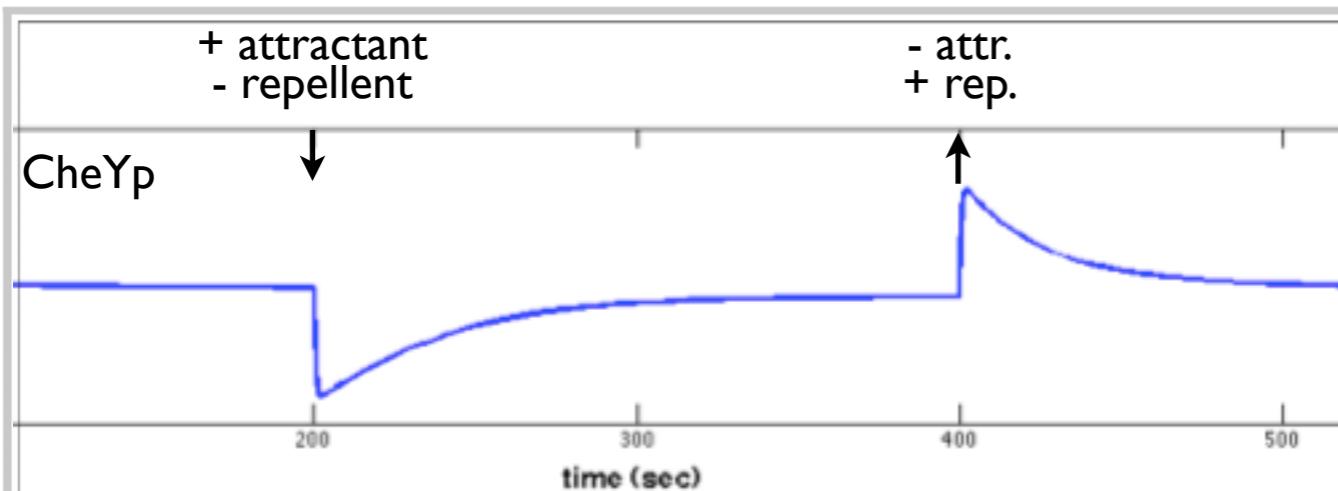
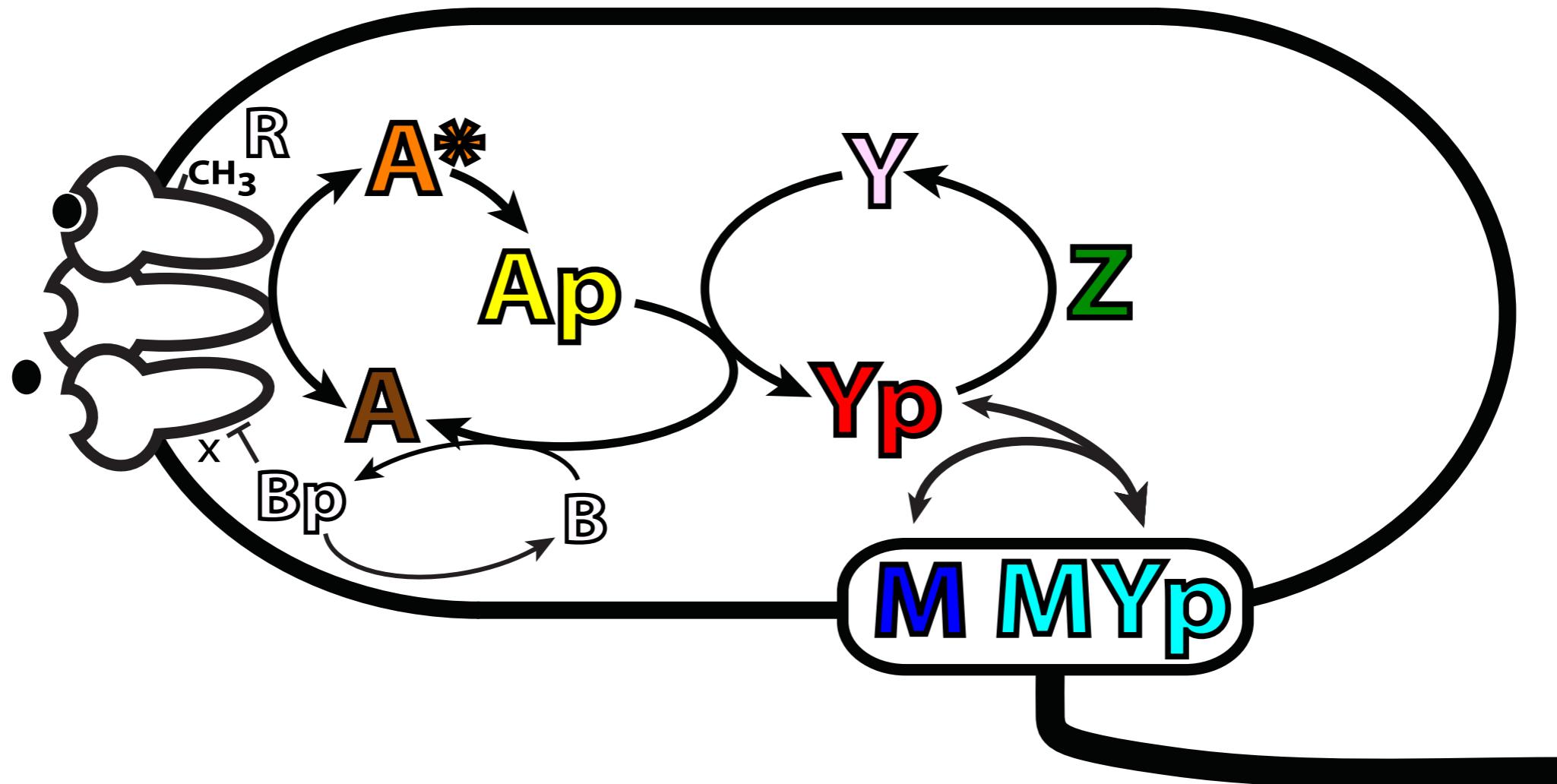
boxsize / molperbox too small: will lead to errors  
boxsize / molperbox too large: inefficient  
timesteps too large for fast reactions

# Swimming *E. coli*



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# The *Escherichia coli* Chemotaxis Pathway



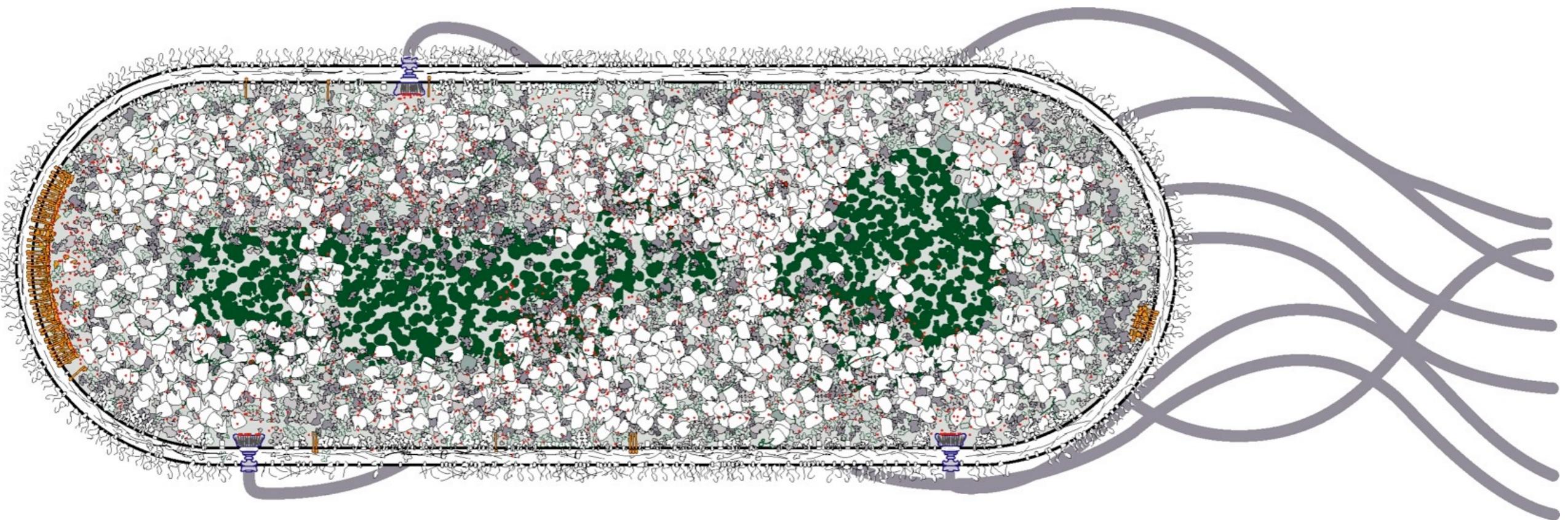
ODE model

Agarwal & Lipkow, unpublished

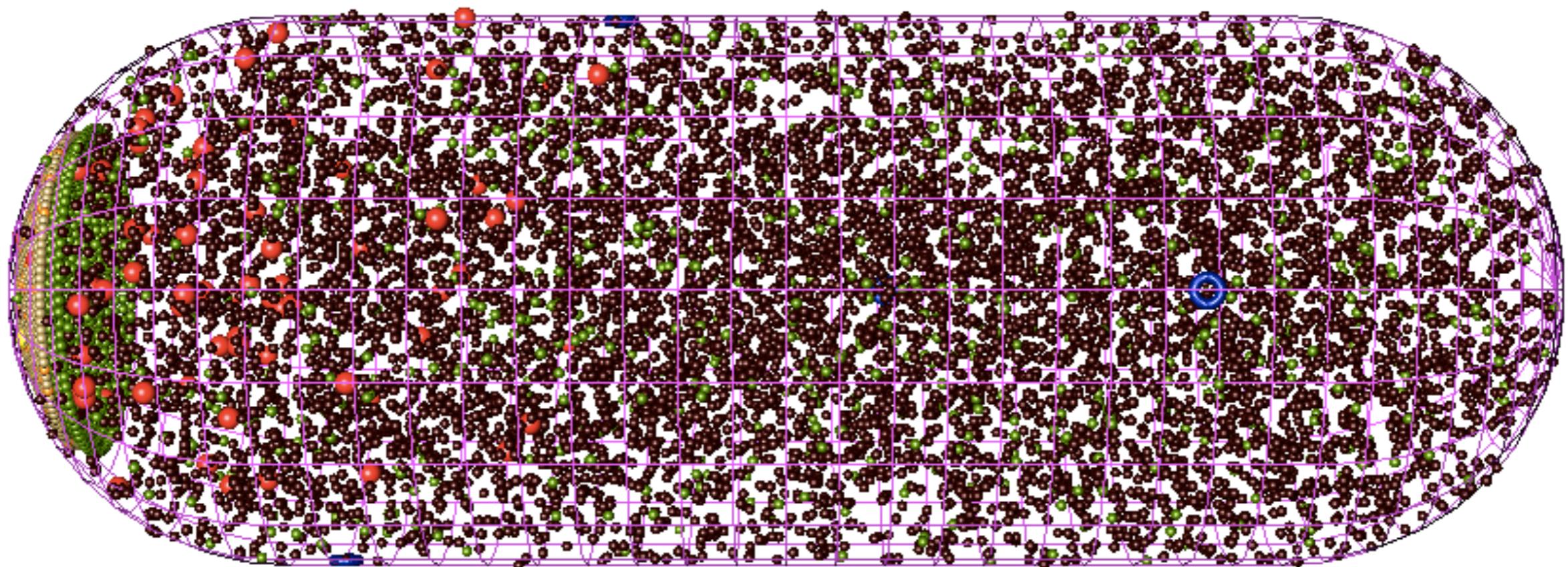
12

Tar, Tsr, Trg, Tap, Aer,  
CheA, CheB, CheR, CheW, CheY, CheZ,  
FliM (Flg, Flh, Fli, Mot)

# Structure of an *Escherichia coli* Cell



# Smoldyn model of an *Escherichia coli* Cell



# Configuration file: Basics

open Smoldyn1/MySims/MySim1.txt

in a text file, enter:

commented title line  
graphics statement:

  opengl\_good

3 dimensions

species:

  A,Am,Ap,Z,Zf,Y,Yp,M,MYp

time: 0-500 ms,  $\Delta t = 0.1$  ms

reflective boundaries (px):

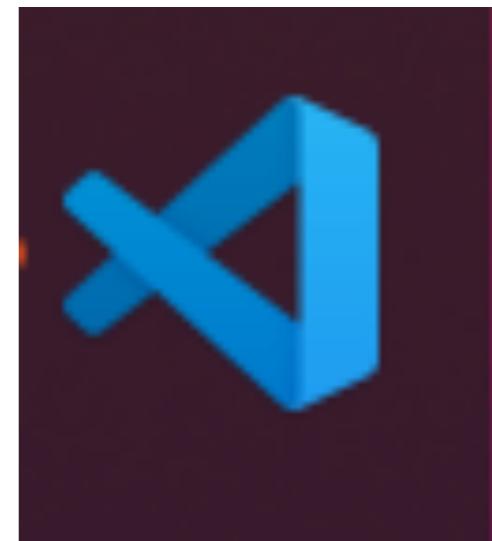
  (x) -50 230

  (y) -50 50

  (z) -50 50

end\_file

Check in  
MIB2\_docs1:  
SmoldynQuickGuide  
SmoldynUsersManual  
  
& as example:  
lotvolt3.txt



Visual Studio Code

# Configuration file: Basics

in a text file, enter:

commented title line  
graphics statement:

**opengl\_good**

3 dimensions

species:

  A,Am,Ap,Z,Zf,Y,Yp,M,MYp

time: 0-500 ms,  $\Delta t = 0.1$  ms

reflective boundaries (px):

  (x) -50 230

  (y) -50 50

  (z) -50 50

end\_file

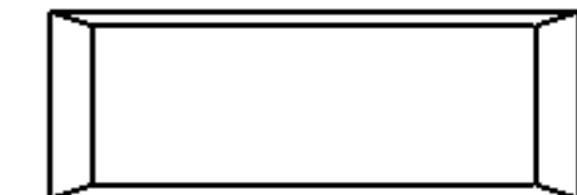
```
# E. coli chemotaxis simulation file for
# graphics opengl_good

dim 3
species A Am Ap Z Zf Y Yp M MYp

time_start 0
time_stop 500
time_step 0.1

boundaries 0 -50 230 r
boundaries 1 -50
boundaries 2 -50

end_file
```



# Configuration file: Molecules

add molecules:

uniformly distributed:

8200 Y

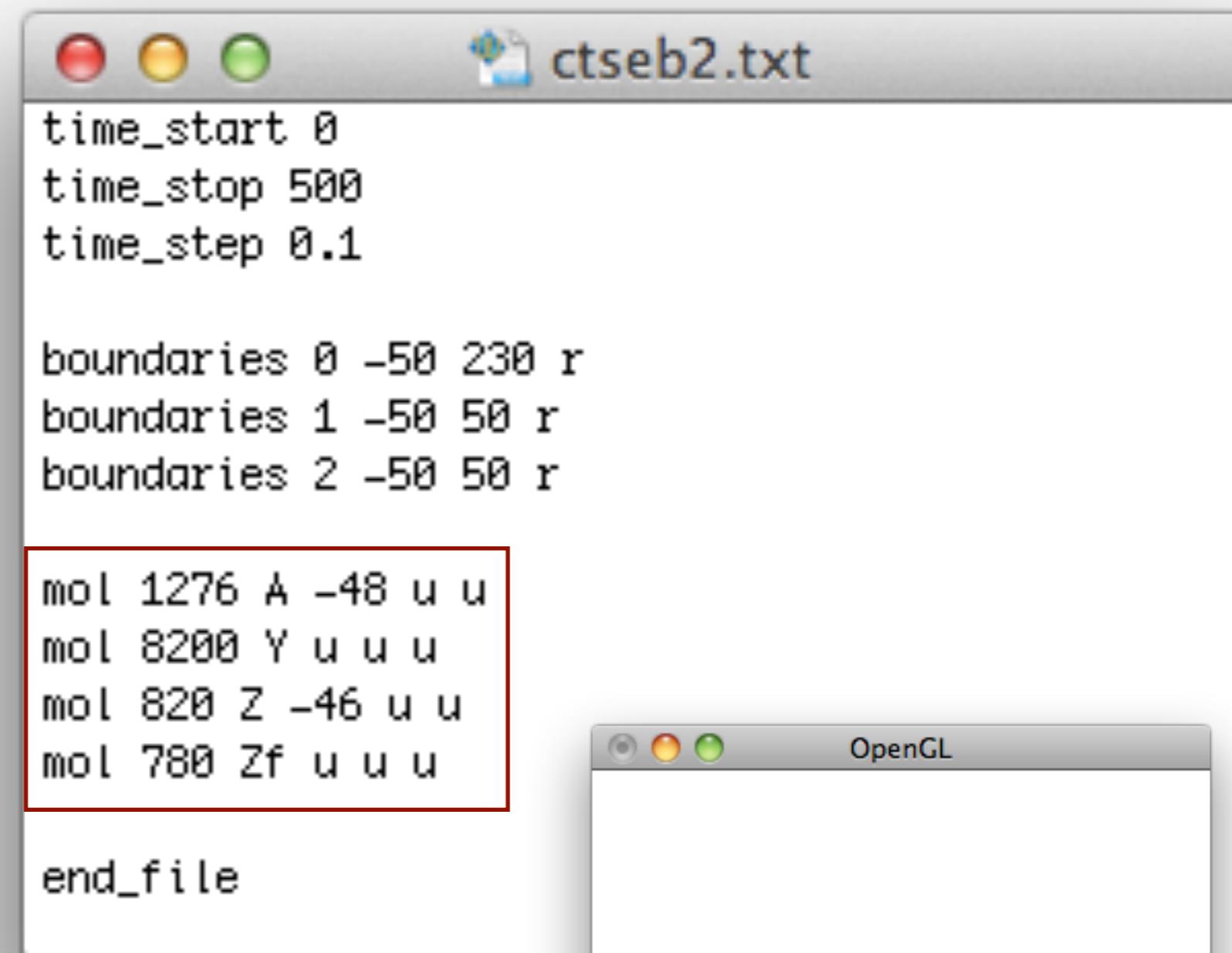
780 Zf

on plane:  $x = -48$

1276 A

on plane:  $x = -46$

820 Z



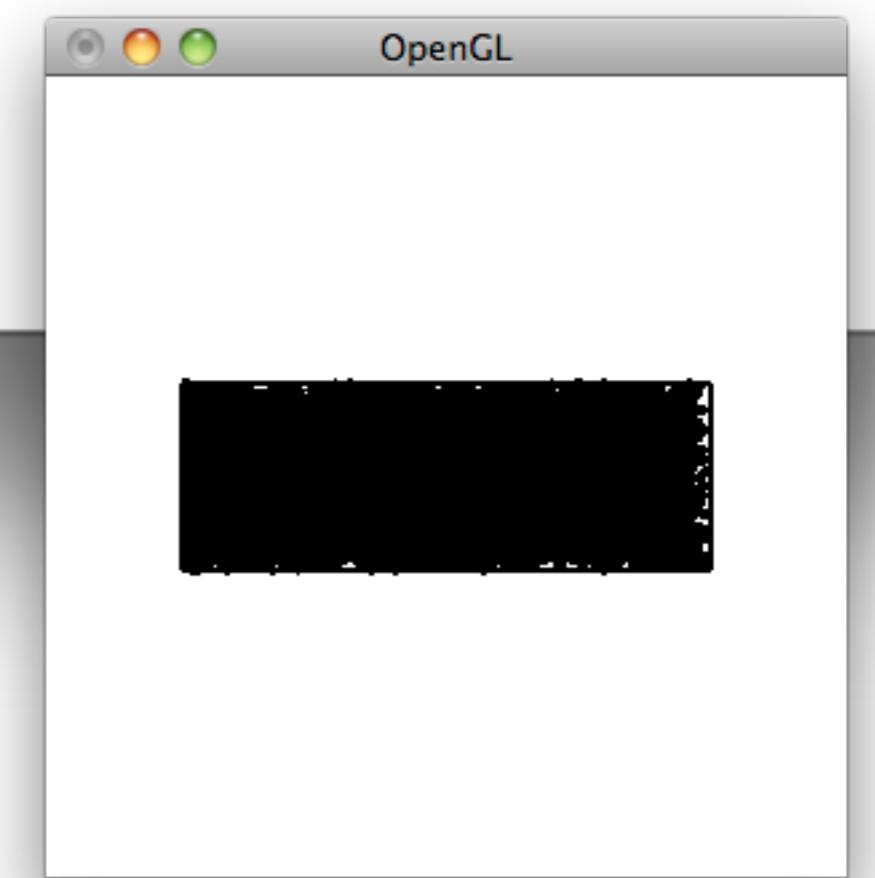
The terminal window shows the contents of the file 'ctseb2.txt'. The file includes parameters for simulation time and boundaries, followed by molecule definitions. The molecule definitions for 'Y' and 'Zf' are highlighted with a red box.

```
time_start 0
time_stop 500
time_step 0.1

boundaries 0 -50 230 r
boundaries 1 -50 50 r
boundaries 2 -50 50 r

mol 1276 A -48 u u
mol 8200 Y u u u
mol 820 Z -46 u u
mol 780 Zf u u u

end_file
```



# Configuration file: Colours and Sizes

colours:

A 0.7 0.6 0.34

Am 1 0.5 0 or orange

Ap 1 1 0 or yellow

Z 0.25 0.5 0

Zf 0.25 0.5 0

Y 0.2 0 0

Yp 1 0 0 or red

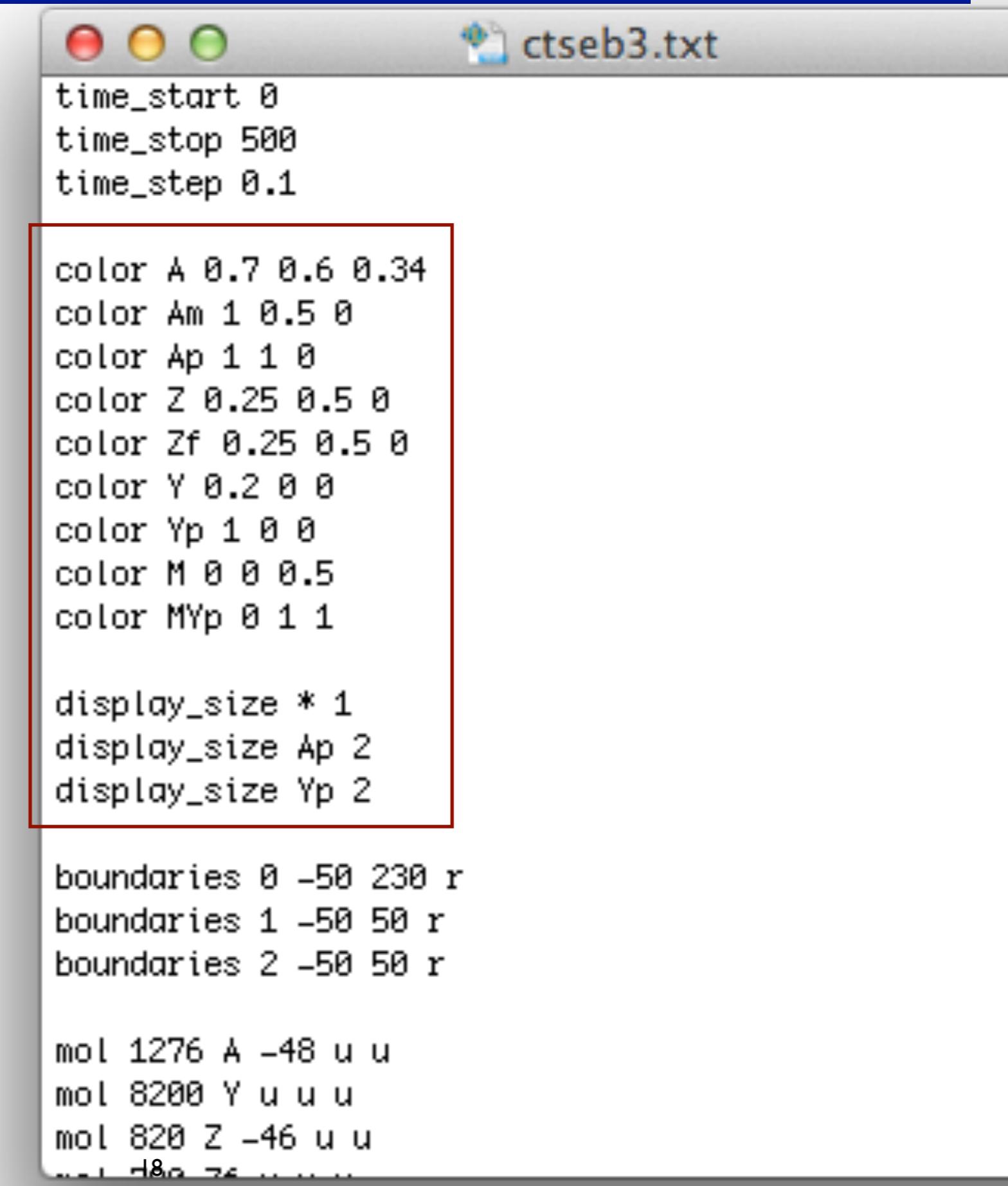
M 0 0 0.5 or blue

MYp 0 1 1 or cyan

display sizes:

Ap and Yp: 2

all others: 1



```
time_start 0
time_stop 500
time_step 0.1

color A 0.7 0.6 0.34
color Am 1 0.5 0
color Ap 1 1 0
color Z 0.25 0.5 0
color Zf 0.25 0.5 0
color Y 0.2 0 0
color Yp 1 0 0
color M 0 0 0.5
color MYp 0 1 1

display_size * 1
display_size Ap 2
display_size Yp 2

boundaries 0 -50 230 r
boundaries 1 -50 50 r
boundaries 2 -50 50 r

mol 1276 A -48 u u
mol 8200 Y u u u
mol 820 Z -46 u u
mol d80 74 u u
```

# Configuration file: Colours and Sizes

```
# E. coli chemotaxis simulation file for EMBL/WT
InSilico

graphics opengl_good

dim 3
species A Am Ap Z Zf Y Yp M MYp

time_start 0
time_stop 500
time_step 0.1

color A 0.7 0.6 0.34
color Am 1 0.5 0
color Ap 1 1 0
color Z 0.25 0.5 0
color Zf 0.25 0.5 0
color Y 0.2 0 0
color Yp 1 0 0
color M 0 0 0.5
color MYp 0 1 1

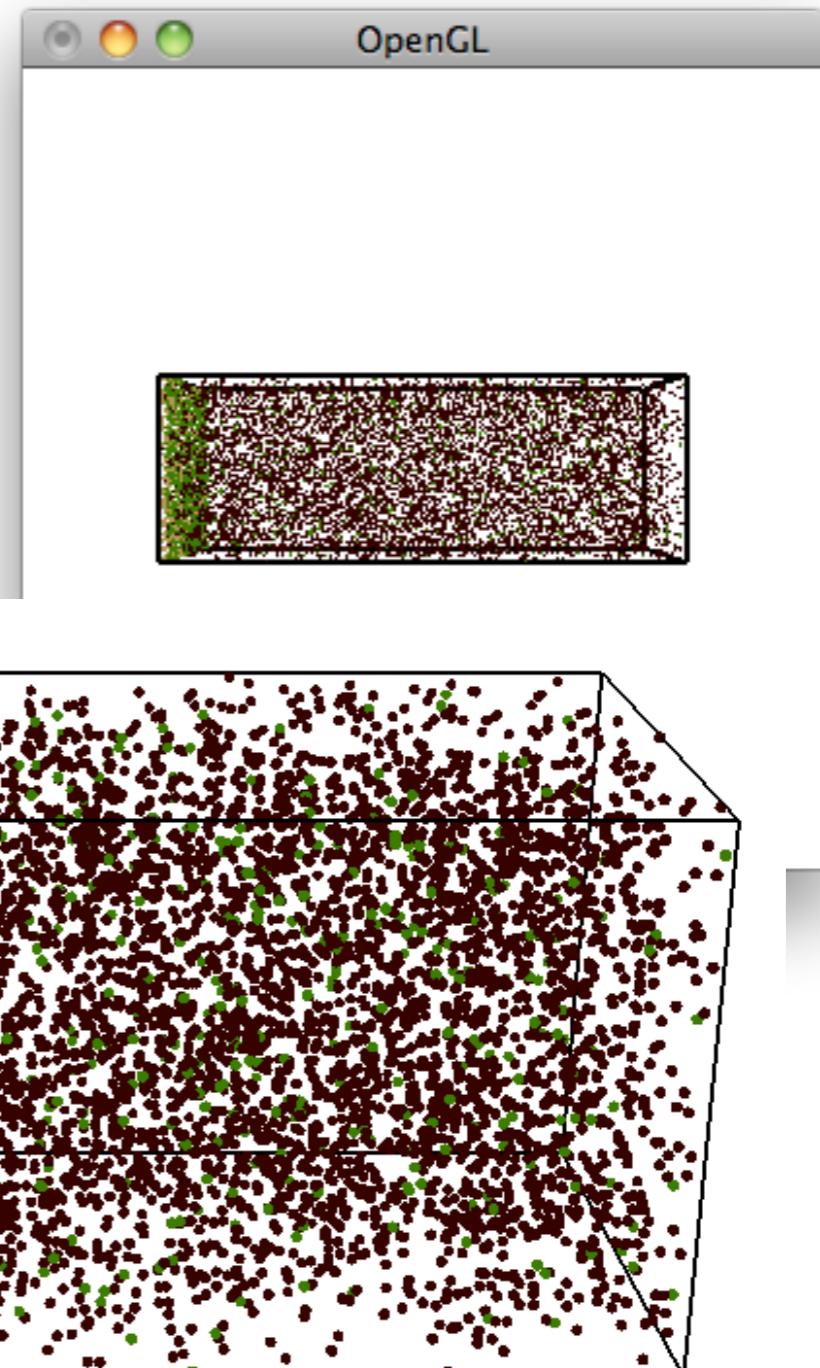
display_size * 1
display_size Ap 2
display_size Yp 2

boundaries 0 -50 230 r
boundaries 1 -50 50 r
boundaries 2 -50 50 r

mol 1276 A -48 u u
mol 8200 Y u u u
mol 820 Z -46 u u
mol 780 Zf u u u

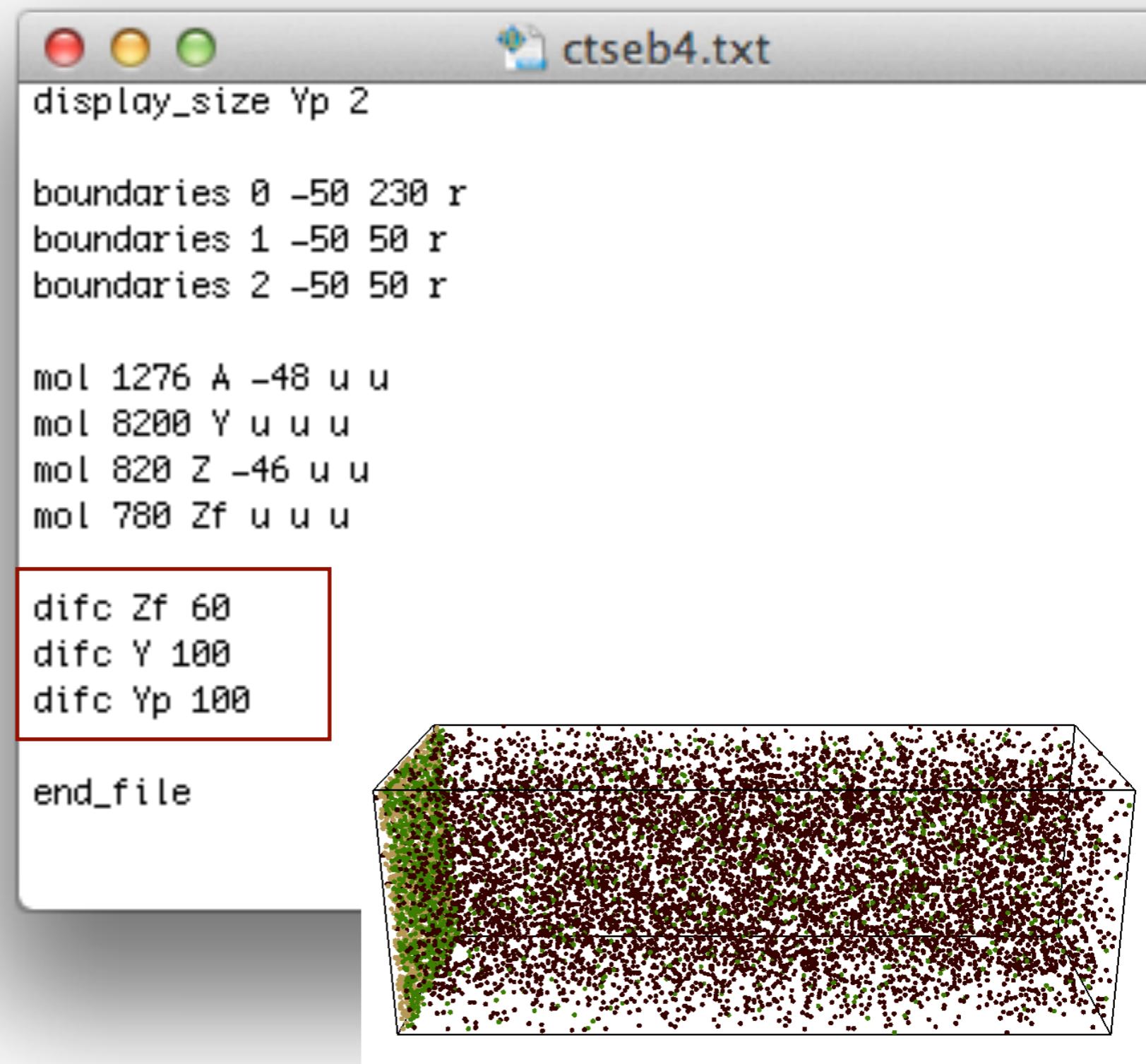
end_file|
```

enlarge window,  
press '=' to zoom in,  
arrows to rotate



# Configuration file: Diffusion

diffusion coefficients:  
Y and Yp 100  
Zf 60  
all others: 0 (default)



```
display_size Yp 2

boundaries 0 -50 230 r
boundaries 1 -50 50 r
boundaries 2 -50 50 r

mol 1276 A -48 u u
mol 8200 Y u u u
mol 820 Z -46 u u
mol 780 Zf u u u

difc Zf 60
difc Y 100
difc Yp 100

end_file
```

## Configuration file: Reactions

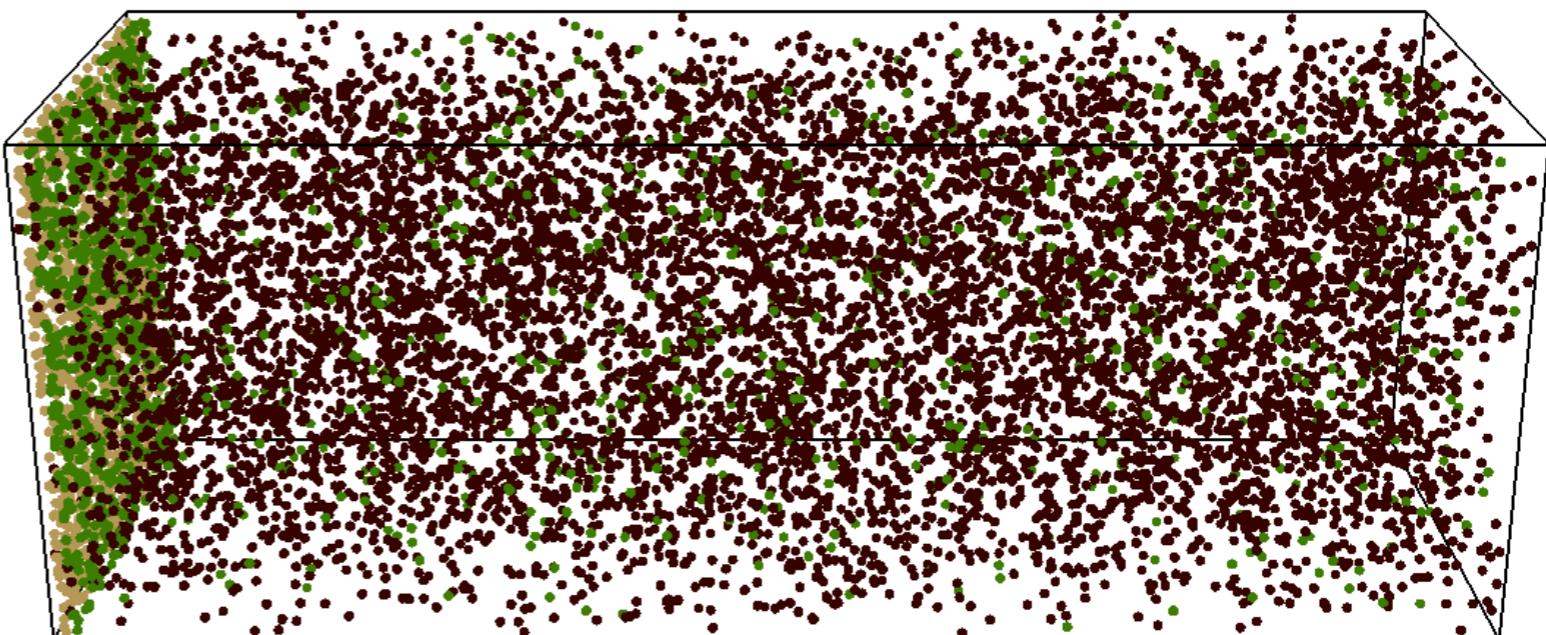
type below difc statements:

```
reaction a1 Am -> Ap           3.4e-2
reaction a2 Y + Ap -> Yp + Am  1.66e2
reaction y1 Y -> Yp            5e-8
reaction y2 Yp -> Y             8.5e-5
reaction m1 Yp + M -> MYp      8.3e0
reaction m2 MYp -> M + Yp      2e-2
product_placement m2 pgemmax 0.2 #optional
reaction z1 Yp + Z -> Y + Z   2.67
reaction z2 Yp + Zf -> Y + Zf  2.67
```

# Configuration file: Reactions

```
mol 8200 Y u u u
mol 820 Z -46 u u
mol 780 Zf u u u

difc Zf 60
difc Y 100
difc Yp 100
```



```
reaction a1 Am -> Ap 3.4e-2
reaction a2 Y + Ap -> Yp + Am 1.66e2
reaction y1 Y -> Yp 5e-8
reaction y2 Yp -> Y 8.5e-5
reaction m1 Yp + M -> MYp 8.3e0
reaction m2 MYp -> M + Yp 2e-2
product_placement m2 pgemmax 0.2
reaction z1 Yp + Z -> Y + Z 2.67
reaction z2 Yp + Zf -> Y + Zf 2.67

end_file
```

# Configuration file: Commands

before simulation start: pause

before simulation start and at  $t = 100$  ms:  
equilibrate A and Am, to have 13% Am

at  $t = 200$  ms:  
equilibrate A and Am, to have 40% Am

```
mol 1270 N -10 u u
mol 8200 Y u u u
mol 820 Z -46 u u
mol 780 Zf u u u

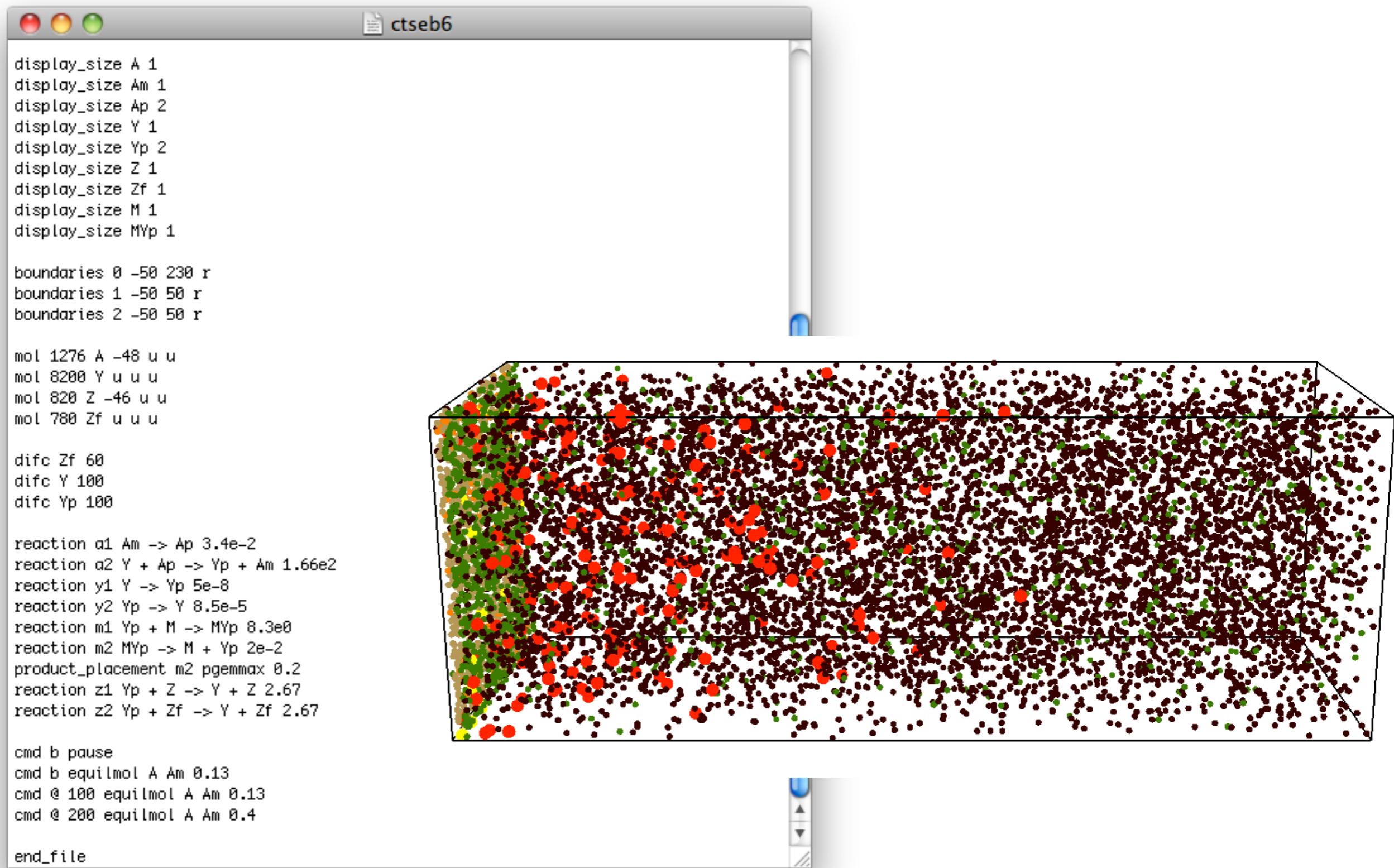
difc Zf 60
difc Y 100
difc Yp 100

reaction a1 Am -> Ap 3.4e-2
reaction a2 Y + Ap -> Yp + Am 1.6e-2
reaction y1 Y -> Yp 5e-8
reaction y2 Yp -> Y 8.5e-5
reaction m1 Yp + M -> MYp 8.3e0
reaction m2 MYp -> M + Yp 2e-2
product_placement m2 pgemmax 0.2
reaction z1 Yp + Z -> Y + Z 2.67
reaction z2 Yp + Zf -> Y + Zf 2.67
```

```
cmd b pause
cmd b equilmol A Am 0.13
cmd @ 100 equilmol A Am 0.13
cmd @ 200 equilmol A Am 0.4
```

```
end_file
```

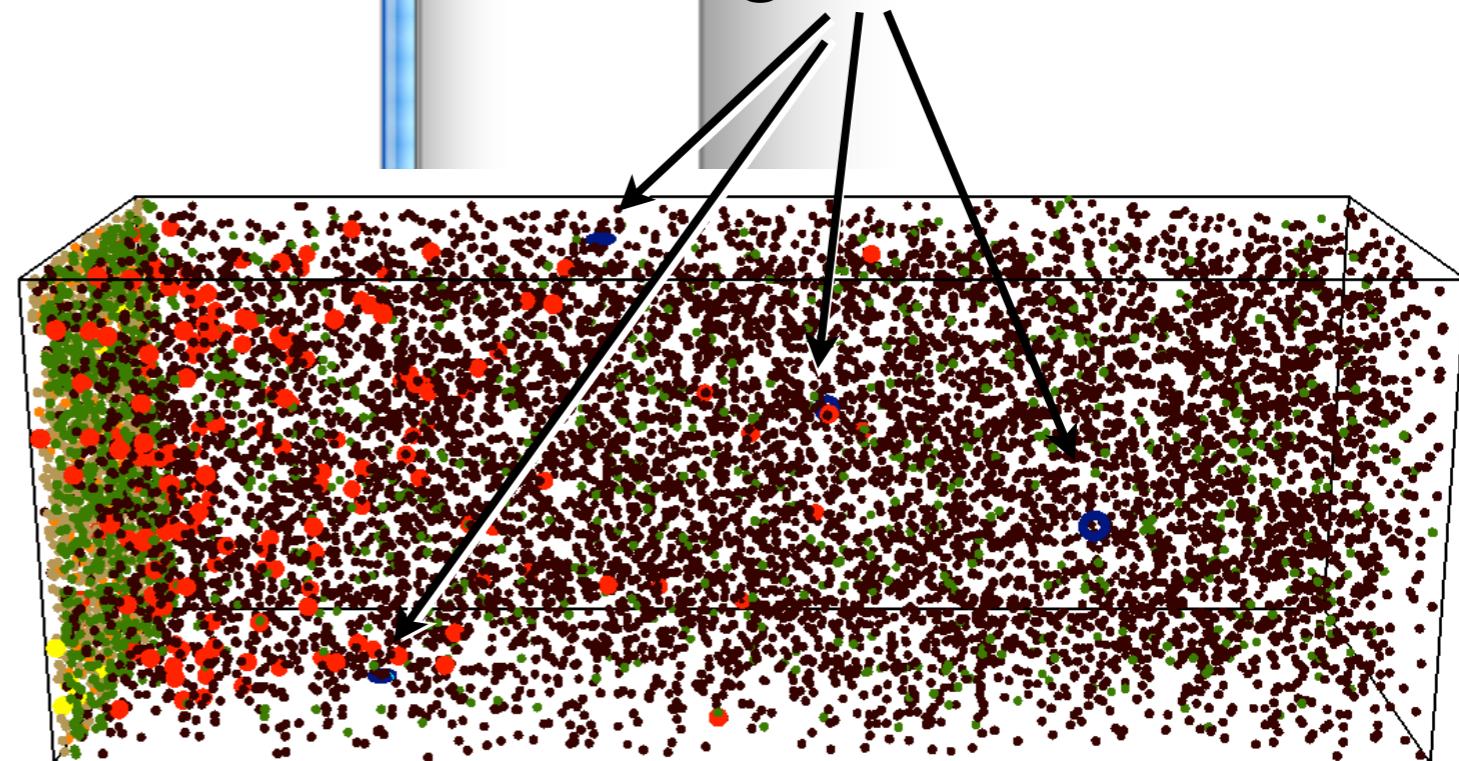
# Configuration file: Commands



# Configuration file: Readfiles

```
boundaries z -50 50 r 10 50 50  
  
mol 1276 A -48 u u  
mol 8200 Y u u u  
mol 820 Z -46 u u  
mol 780 Zf u u u  
read_file posE_M_49  
  
difc Zf 60  
difc Y 100  
difc Yp 100  
  
reaction a1 Am -> Ap 3.4e-  
reaction a2 Y + Ap -> Yp +  
reaction y1 Y -> Yp 5e-8  
reaction y2 Yp -> Y 8.5e-5  
reaction m1 Yp + M -> MYp  
reaction m2 MYp -> M + Yp  
product_placement m2 pgemn  
reaction z1 Yp + Z -> Y +  
reaction z2 Yp + Zf -> Y +  
  
cmd b pause  
cmd b equilmol A Am 0.13  
cmd @ 100 equilmol A Am 0.  
cmd @ 200 equilmol A Am 0.  
  
mol 1 M 12.250000 -49 0.000000  
mol 1 M 12.211689 -49 0.413436  
mol 1 M 12.098063 -49 0.812794  
mol 1 M 11.912989 -49 1.184472  
mol 1 M 11.662770 -49 1.515815  
mol 1 M 11.355928 -49 1.795539  
mol 1 M 11.002911 -49 2.014117  
mol 1 M 10.615742 -49 2.164108  
mol 1 M 10.207604 -49 2.240402  
mol 1 M 9.792396 -49 2.240402  
mol 1 M 9.384258 -49 2.164108  
mol 1 M 8.997089 -49 2.014117  
mol 1 M 8.644072 -49 1.795539  
mol 1 M 8.337230 -49 1.515815  
mol 1 M 8.087011 -49 1.184472  
mol 1 M 7.901937 -49 0.812794  
mol 1 M 7.788311 -49 0.413436  
mol 1 M 7.750000 -49 0.000000  
mol 1 M 7.788311 -49 -0.413436  
mol 1 M 7.901937 -49 -0.812794  
mol 1 M 8.087011 -49 -1.184472  
mol 1 M 8.337230 -49 -1.515815  
mol 1 M 8.644072 -49 -1.795539  
mol 1 M 8.997089 -49 -2.014117  
mol 1 M 9.384258 -49 -2.164108  
mol 1 M 9.792396 -49 -2.240402  
mol 1 M 10.207604 -49 -2.240402  
mol 1 M 10.615742 -49 -2.164108  
mol 1 M 11.002911 -49 -2.014117  
mol 1 M 11.355928 -49 -1.795539  
mol 1 M 11.662770 -49 -1.515815  
mol 1 M 11.912989 -49 -1.184472  
mol 1 M 12.098063 -49 -0.812794  
mol 1 M 12.211689 -49 -0.413436  
mol 1 M 62.250000 49 0.000000  
mol 1 M 62.211689 49 0.413436  
mol 1 M 62.098063 49 0.812794  
mol 1 M 61.912989 49 1.184472  
mol 1 M 61.662770 49 1.515815  
mol 1 M 61.355928 49 1.795539  
mol 1 M 61.002911 49 2.014117
```

4 motors:  
rings of 34 FliM



molecule array files generated with  
C, Perl, Python, etc.

# Configuration file: Readfiles

replace random  
CheA and CheZ  
clusters with  
ordered, curved  
arrays

```
boundaries 2 -50 50 r

# mol 1276 A -48 u u
read_file posE_A_48_1.5_1276
mol 8200 Y u u u
# mol 820 Z -46 u u
read_file posE_Z_46_2_820
mol 780 Zf u u u
read_file posE_M_49

difc Zf 60
difc Y 100
difc Yp 100

reaction a1 Am ->
reaction a2 Y + +
reaction y1 Y ->
```

# Configuration file: Surfaces

Add cell membrane as *E. coli*-shaped surface, filling the boundaries.

It helps to:

- initially choose graphics opengl (instead of opengl\_good) to make molecules appear smaller
- look at the surfaces before starting the simulation (don't hit the space bar)

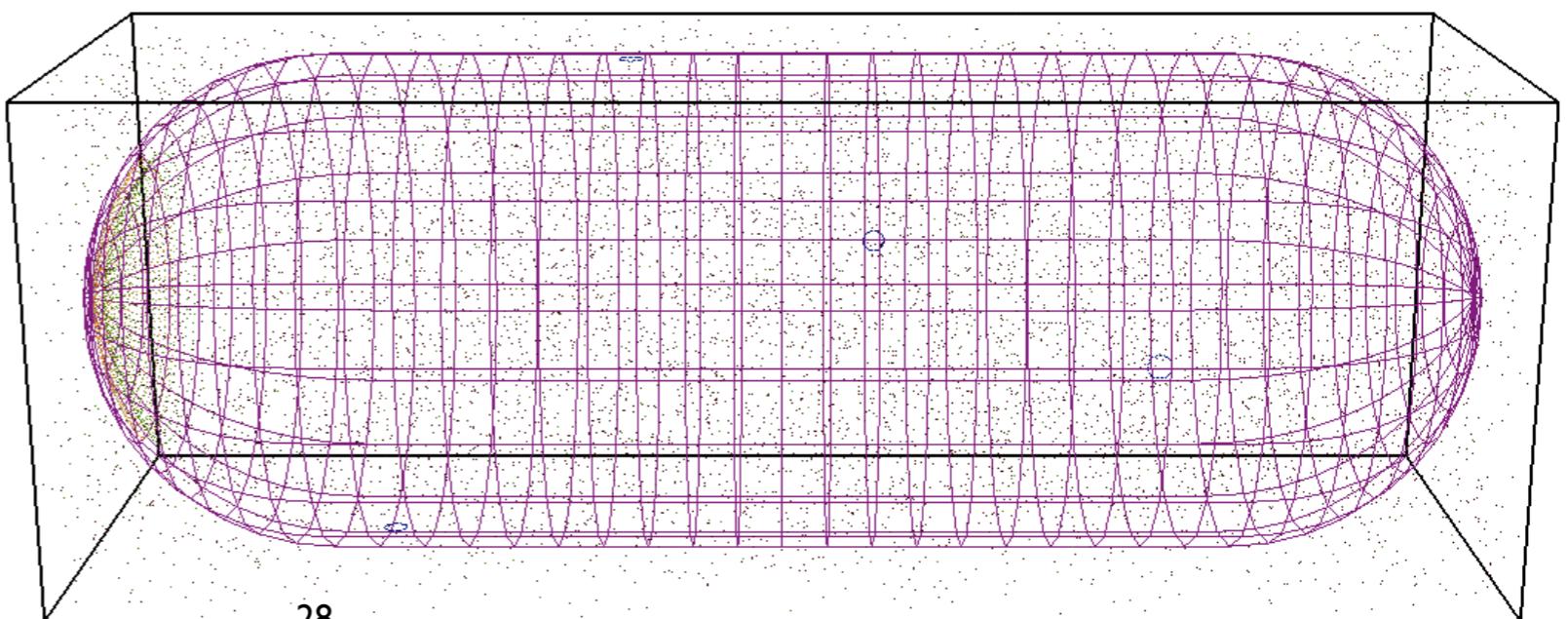
Two polar hemispheres, one cylinder; reflective.

Hint: SmodynManual p. 127ff

# Configuration file: Surfaces

Add cell membrane as *E. coli*-shaped surface, filling the boundaries.

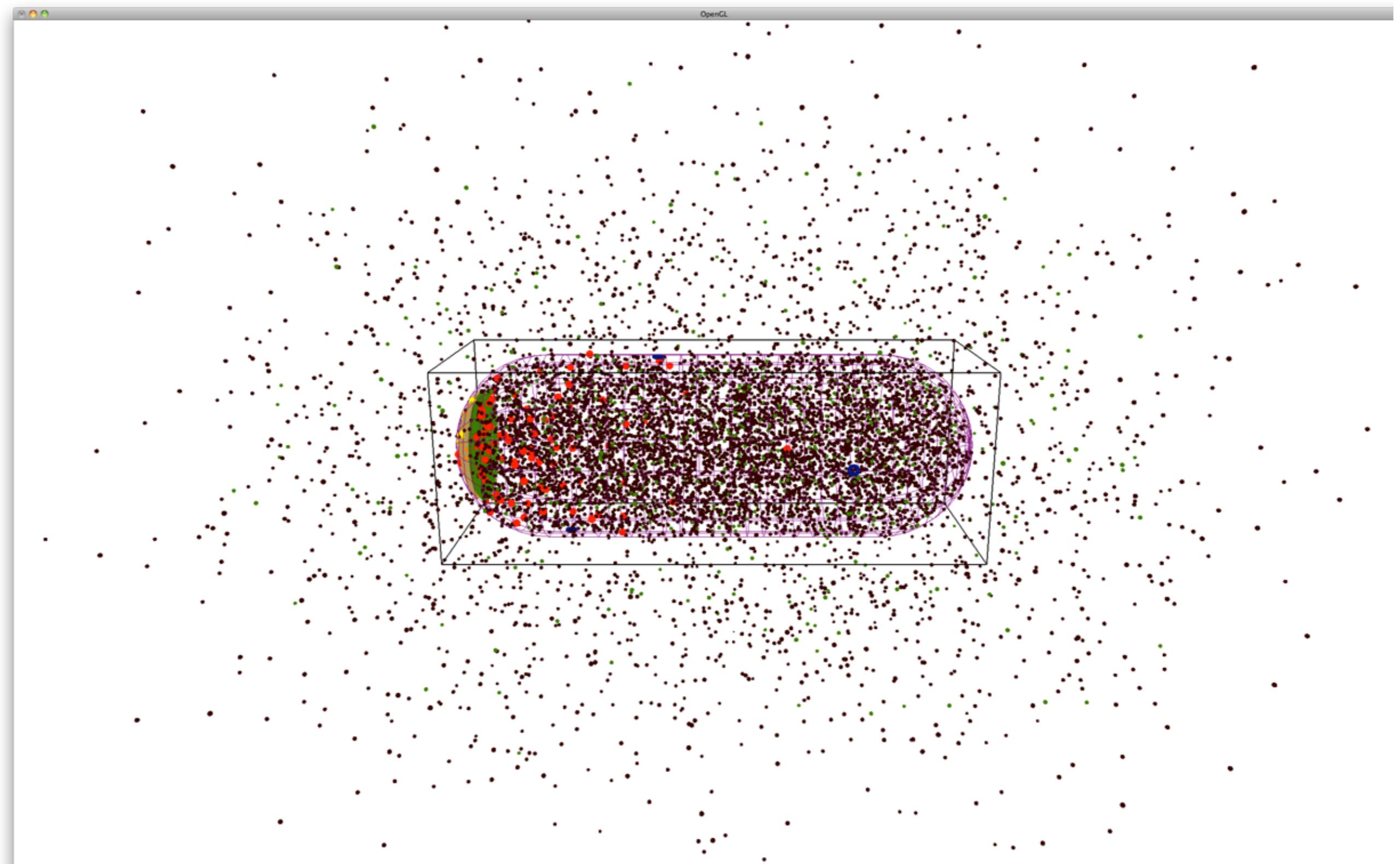
```
start_surface cellmembrane
  action all both reflect
  color both purple 1
  polygon both edge
  panel hemi 0 0 0 50 1 0 0 20 10
  panel hemi 180 0 0 50 -1 0 0 20 10
  panel cyl 0 0 0 180 0 0 50 20 20
end_surface
```



# Configuration file: Surfaces

return to good graphics and start simulation...

# Configuration file: Surfaces



If model includes surfaces, boundaries transmit.

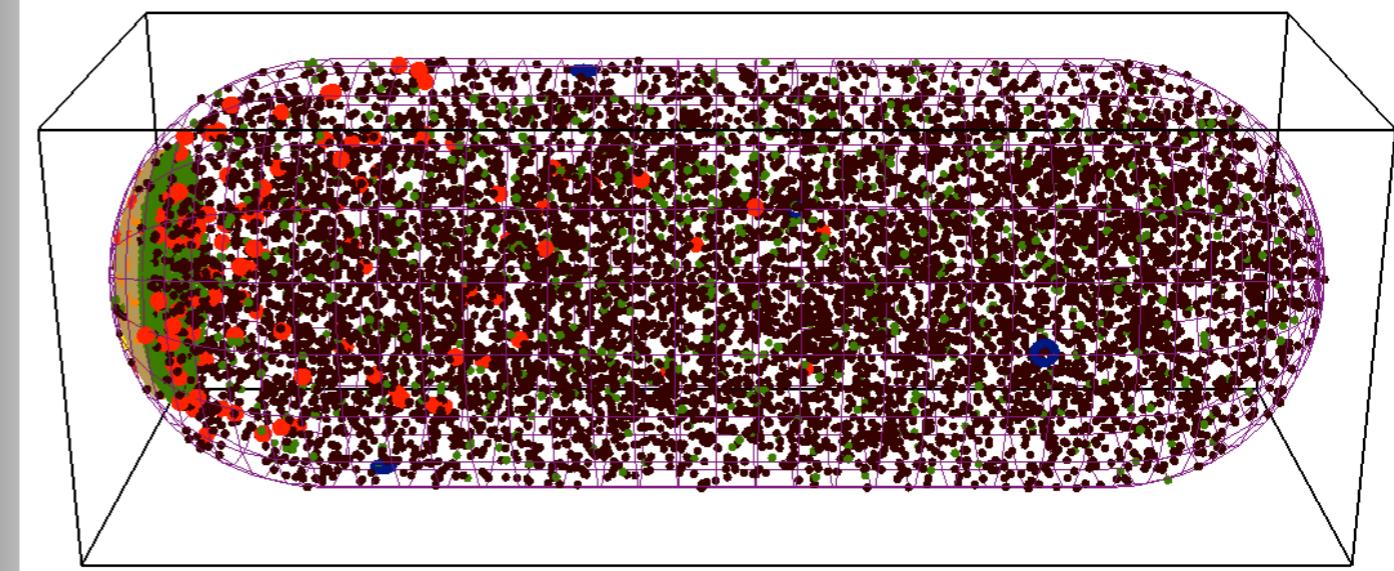
# Configuration file: Compartments

make a compartment "cytoplasm"  
place diffusing molecules into this compartment

```
start_surface cellmembrane
action all both reflect
color both purple 1
polygon both edge
panel hemi 0 0 0 50 1 0 0 20 10
panel hemi 180 0 0 50 -1 0 0 20 10
panel cyl 0 0 0 180 0 0 50 20 20
end_surface

start_compartment cytoplasm
surface cellmembrane
point 100 0 0
end_compartment

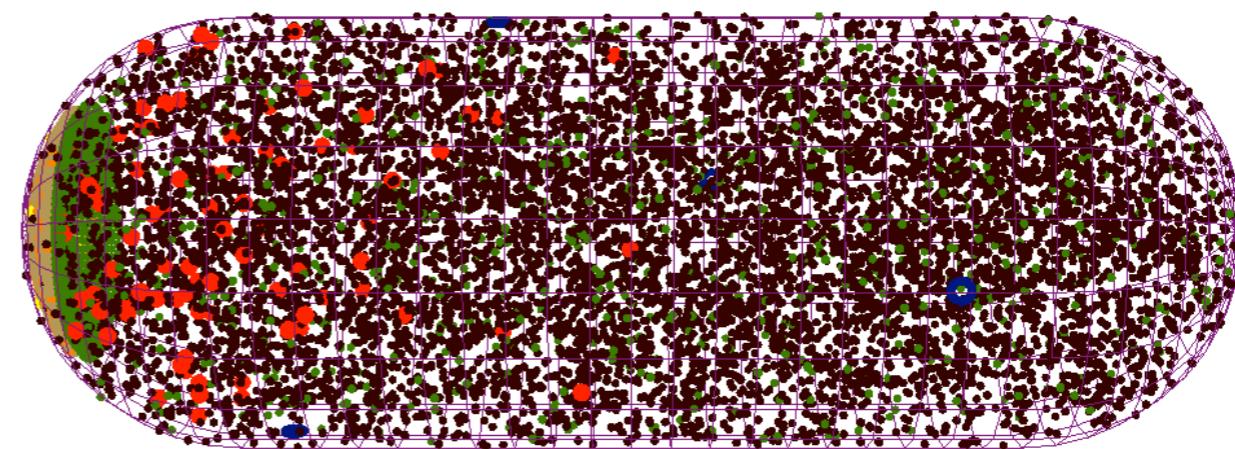
# mol 1276 A -48 u u
read_file posE_A_48_1.5_1276
# mol 8200 Y u u u
compartment_mol 8200 Y cytoplasm
# mol 820 Z -46 u u
read_file posE_Z_46_2_820
# mol 780 Zf u u u
compartment_mol 780 Zf cytoplasm
read_file posE_M_49
```



# Configuration file: better Graphics

remove the frame

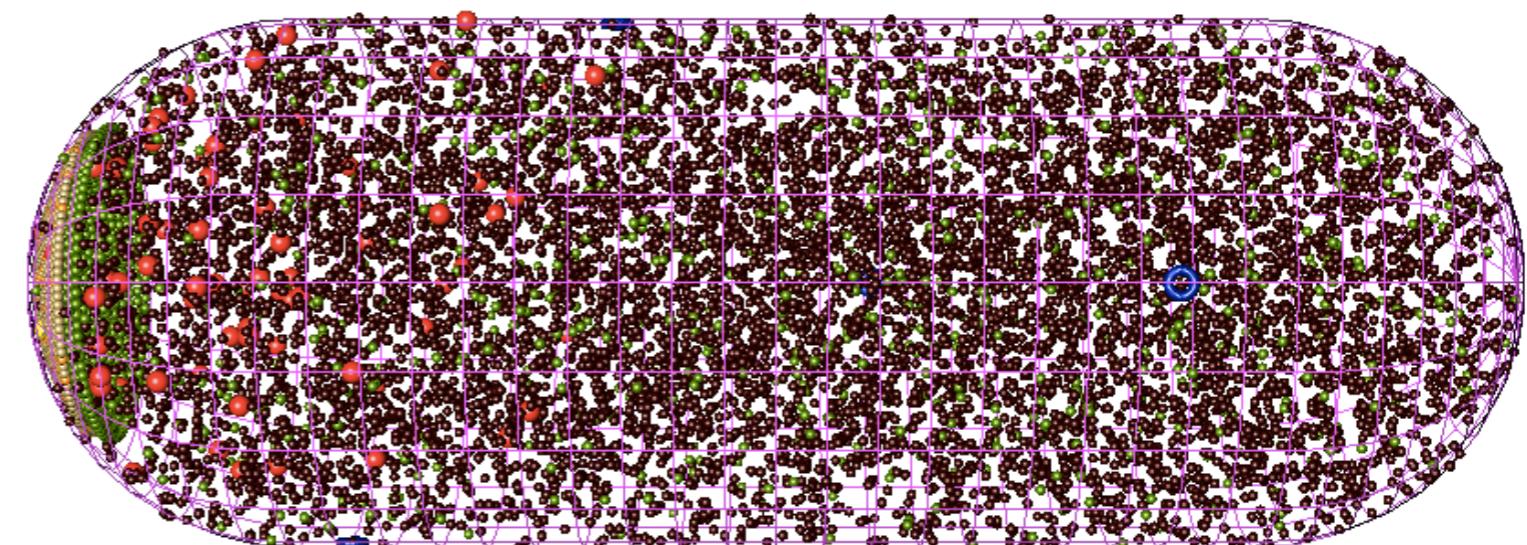
```
ctseb12.txt — Edited  
# E. coli chemotaxis simulation file for SEB3.2  
  
# graphics opengl  
# graphics opengl_good  
graphics opengl_better  
  
frame_thickness 0  
  
background_color 1 1 1  
light 0 position -50 50 0  
light 0 diffuse 1 1 1  
light 0 ambient 0.05 0.05 0.05  
light 0 specular 1 1 1  
  
dim 3  
species A Am Ap Z Zf Y Yp M MYp
```



# Configuration file: better Graphics

improve graphics

```
ctseb12.txt — Edited  
# E. coli chemotaxis simulation file for SEB3.2  
  
# graphics opengl  
# graphics opengl_good  
graphics opengl_better  
  
frame_thickness 0  
  
background_color 1 1 1  
light 0 position -50 50 0  
light 0 diffuse 1 1 1  
light 0 ambient 0.05 0.05 0.05  
light 0 specular 1 1 1  
  
dim 3  
species A Am Ap Z Zf Y Yp M MYp
```



# Observation commands: molcount

create output file and count number  
of all molecules at 10 ms intervals

```
# E. coli chemotaxis simulation file for SEB3.2

# graphics opengl_good
# graphics opengl

dim 3
species A Am Ap Z Zf Y Yp M MYp
max_mol 20000
# boxsize 15

time_start 0
time_stop 6000
time_step 1

color A 0.7 0.6 0.34
color Am 1 0.5 0
color Ap 1 1 0
color Z 0.25 0.5 0
color Zf 0.25 0.5 0
color Y 0.2 0 0
color Yp 1 0 0
color M 0 0 0.5
color MYp 0 1 1

display_size A 1
display_size Am 1
display_size Ap 2
display_size Y 1
display_size Yp 2
display_size Z 1
display_size Zf 1
display_size M 1
display_size MYp 1

boundaries 0 -50 230 r
boundaries 1 -50 50 r
boundaries 2 -50 50 r

# frame_thickness 0

start_surface cellmembrane|
action all both reflect
```

```
ctseb13

end_compartment

# mol 1276 A -48 u u
read_file posE_A_48_1.5_1276
# mol 8200 Y u u u
compartment_mol 8200 Y cytoplasm
# mol 820 Z -46 u u
read_file posE_Z_46_2_820
# mol 780 Zf u u u
compartment_mol 780 Zf cytoplasm
read_file posE_M_49

difc Zf 60
difc Y 100
difc Yp 100

reaction a1 Am -> Ap 3.4e-2
reaction a2 Y + Ap -> Yp + Am 1.66e2
reaction y1 Y -> Yp 5e-8
reaction y2 Yp -> Y 8.5e-5
reaction m1 Yp + M -> MYp 8.3e0
reaction m2 MYp -> M + Yp 2e-2
product_placement m2 pgemmax 0.2
reaction z1 Yp + Z -> Y + Z 2.67
reaction z2 Yp + Zf -> Y + Zf 2.67

/*
cmd b pause
cmd b equilmol A Am 0.13
cmd @ 100 equilmol A Am 0.13
cmd @ 200 equilmol A Am 0.4
*/
cmd i 0 1990 10 equilmol A Am 0.132
cmd i 2000 3990 10 equilmol A Am 0.066
cmd i 4000 5990 10 equilmol A Am 0.132

output_files out2.txt
cmd i 0 1000000 10 molcount out2.txt

end_file
```

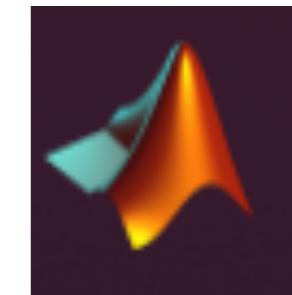
remove all (!) graphics  
time step 1 ms

```
out2.txt

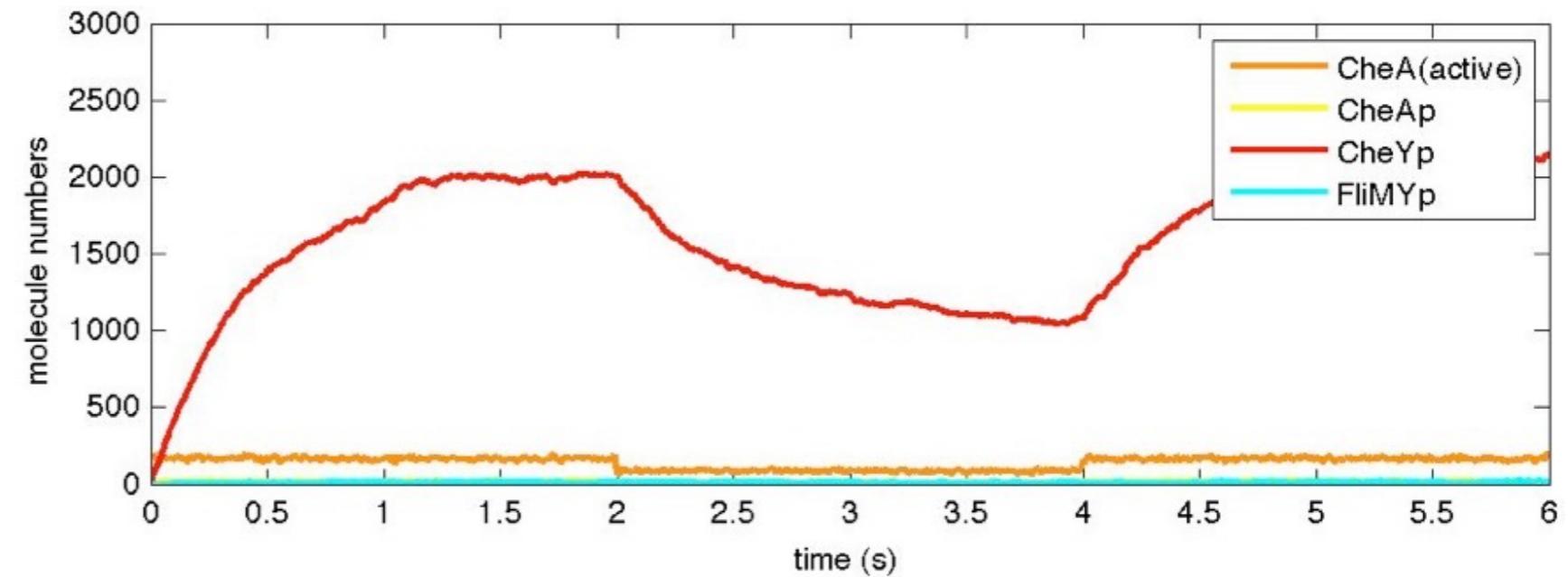
0 1101 175 0 820 780 8200 0 136 0
10.1 1070 197 9 820 780 8156 44 136 0
20 1087 177 12 820 780 8118 82 136 0
30 1101 165 10 820 780 8078 122 136 0
40 1104 167 5 820 780 8041 159 136 0
50 1115 159 2 820 780 8004 196 136 0
60 1108 160 8 820 780 7975 225 136 0
70 1074 193 9 820 780 7943 257 136 0
80.1 1097 167 12 820 780 7892 308 136 0
90.1 1083 177 16 820 780 7852 347 135 1
100.1 1088 176 12 820 780 7819 380 135 1
110.1 1094 168 14 820 780 7779 418 133 3
120.1 1093 171 12 820 780 7746 450 132 4
130.1 1101 163 12 820 780 7699 496 131 5
140.1 1098 169 9 820 780 7658 536 130 6
150.1 1092 180 4 820 780 7624 569 129 7
160.1 1084 173 19 820 780 7609 583 128 8
170.1 1074 188 14 820 780 7566 628 130 6
180.1 1101 164 11 820 780 7536 657 129 7
190.1 1116 152 8 820 780 7506 687 129 7
200.1 1178 83 15 820 780 7483 709 128 8
210.1 1201 73 2 820 780 7475 716 127 9
220.1 1199 77 0 820 780 7484 704 124 12
230.1 1179 95 2 820 780 7484 707 127 9
240.1 1182 88 6 820 780 7474 718 128 8
250.1 1198 71 7 820 780 7470 719 125 11
260.1 1181 91 4 820 780 7455 732 123 13
270.1 1171 96 9 820 780 7464 722 122 14
280.1 1189 81 6 820 780 7466 723 125 11
290.1 1197 77 2 820 780 7465 719 120 16
300.1 1177 93 6 820 780 7459 727 122 14
310 1191 81 4 820 780 7447 739 122 14
```

# Observation commands: molcount

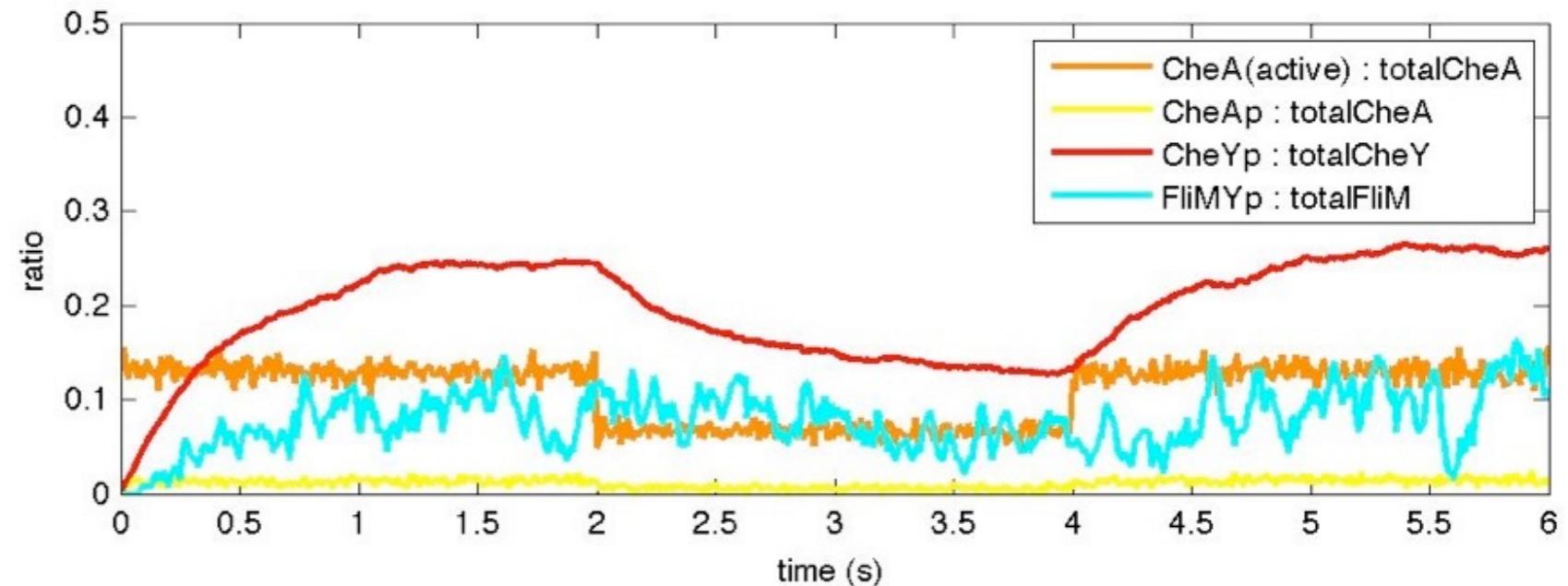
start MATLAB from desktop icon or from a new terminal window: type matlab



plot and convert using MATLAB:  
`Mctseb.m`



move `Mctseb.m` from Smoldyn1/m-files to MyFiles



## More quantitative simulations

*(If you still have time, otherwise continue tomorrow.)*

Create a new folder for each new simulation

# Preparation for spatial distribution

to get a more pronounced Yp gradient, make all Z diffusible

```
# read_file posE_Z_46_2_820  
# mol 780 Zf u u u  
compartment_mol 1600 Zf cytoplasm
```

to let the cell reach steady state, change the CheA activation profile to always have on average 13.2% Am

```
#cmd i 2000 3990 10 equilmol A Am 0.066  
#cmd i 4000 5990 10 equilmol A Am 0.132  
cmd i 0 5990 10 equilmol A Am 0.132
```

record time profile of molecule numbers to check when steady state is reached

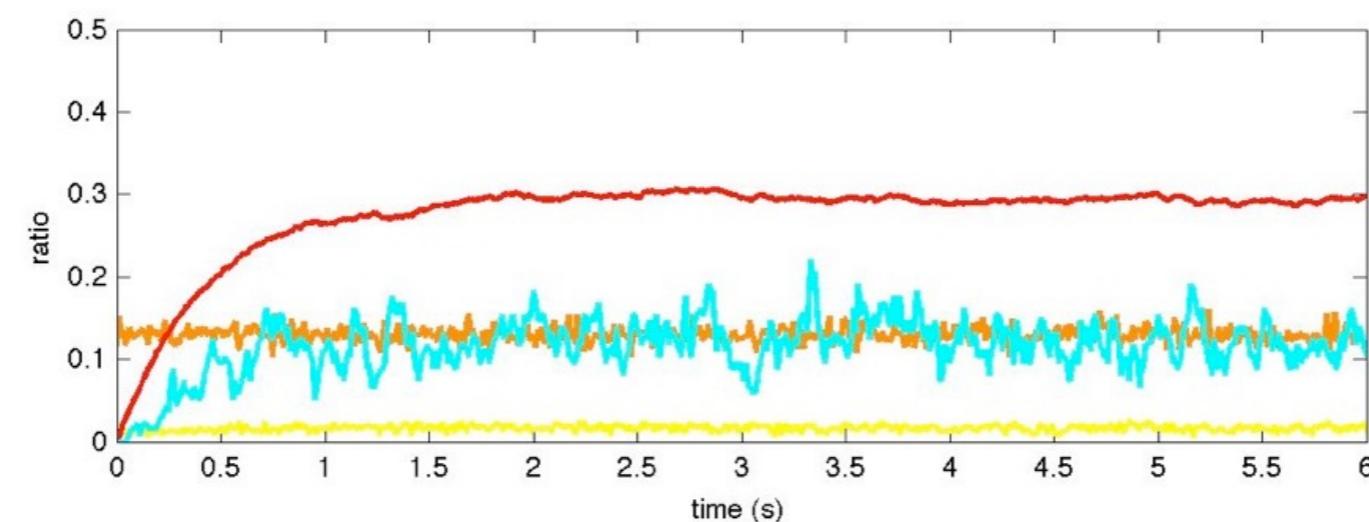
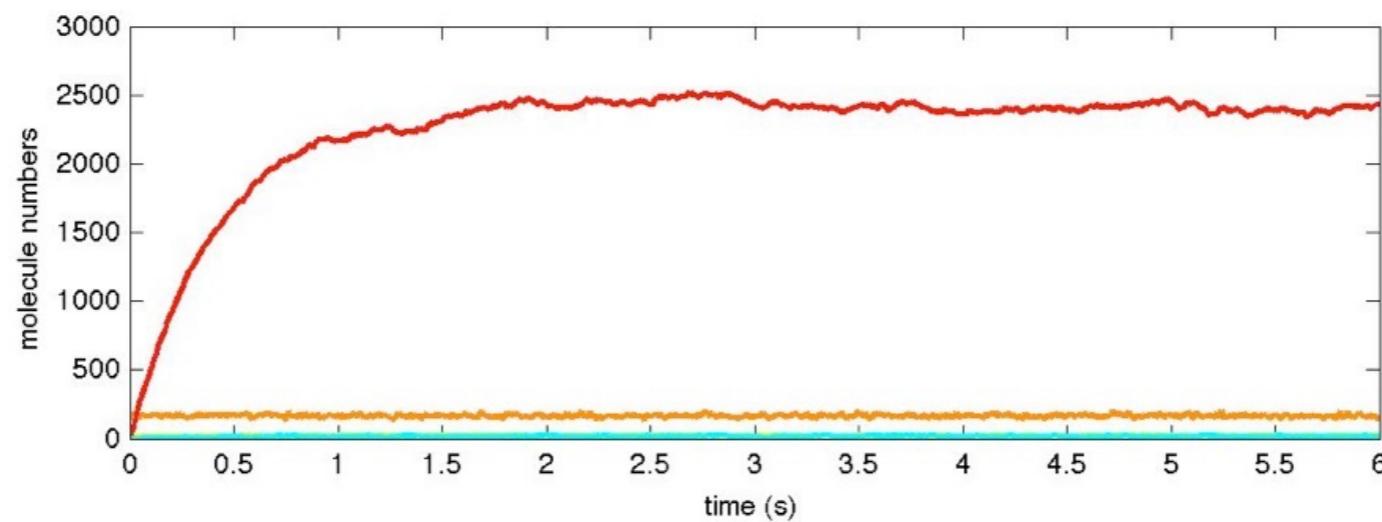
```
output_files out2.txt  
cmd n 10 molcount out2.txt
```

plot with MATLAB

Mctseb.m

# Time profile

molcount (out2) / Mctseb.m: steady state reached at c. t = 2000 ms



# Configuration file: Record spatial distribution

change duration to sensible time

```
time_stop 3000
```

record histograms of the spatial distribution of Yp along the x-axis:

100 snapshots every 10 ms at steady state

30 x 100ms-averages during buildup

```
output_files out2.txt out3_Yp.txt out4_Yp.txt
```

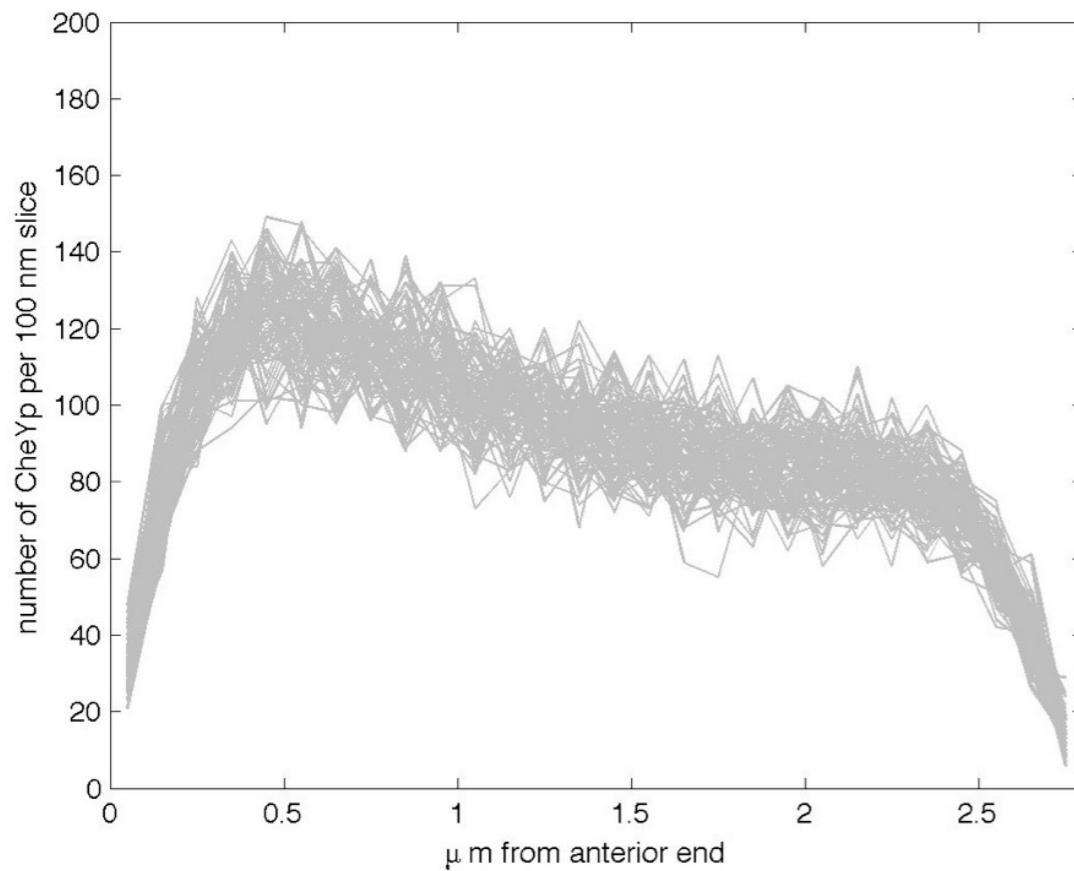
```
cmd n 10 molcount out2.txt
```

```
cmd i 2000 3000 10 molcountsphere Yp 0 -50 230 28 -50 50 -50 50 0 out3_Yp.txt
```

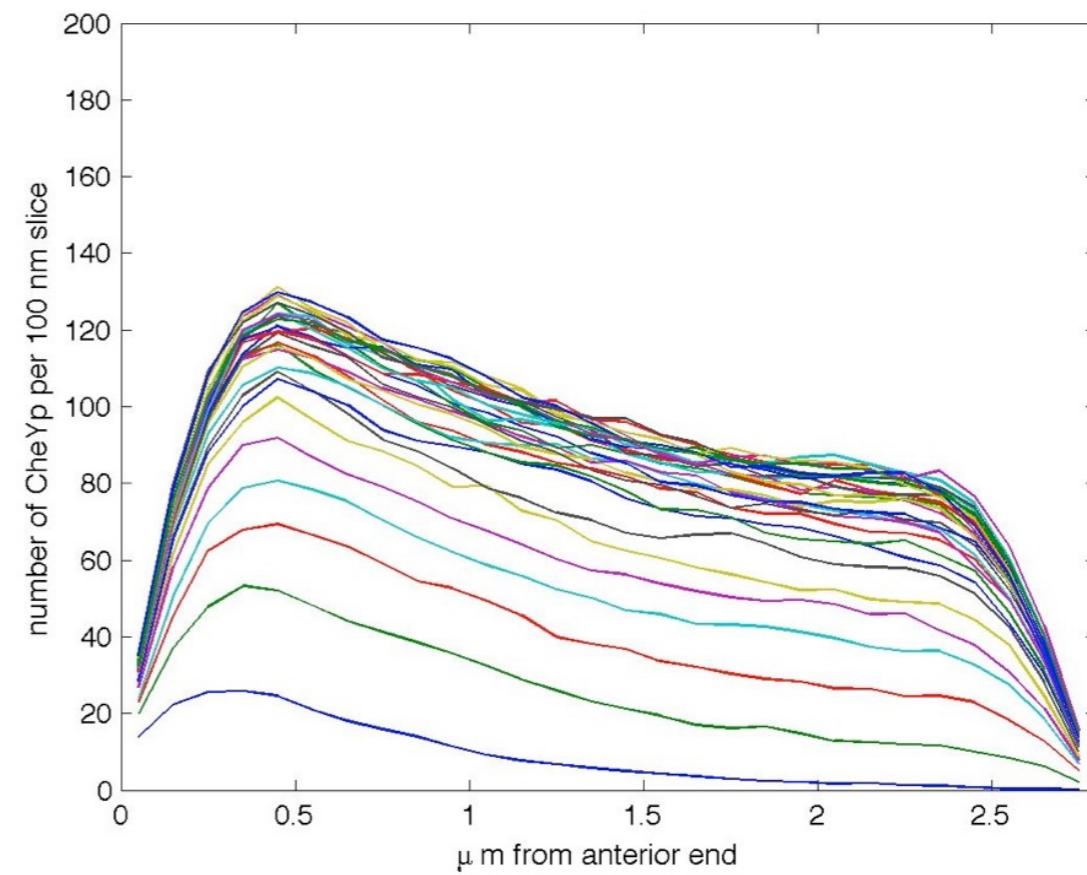
```
cmd i 0 3000 1 molcountsphere Yp 0 -50 230 28 -50 50 -50 50 100 out4_Yp.txt
```

# Spatial distribution

molcountspace (out3\_Yp) / Yprofile.m:  
snapshots at steady state (2000-3000 ms)



molcountspace (out4\_Yp) / YprofileTime.m:  
100ms-averages during Yp buildup (0-3000 ms)



# Spatial distribution

to normalise for total CheY concentration and varying volume along the x-axis,  
also record profile of Y molecules

```
output_files out2.txt out3_Yp.txt out3_Y.txt out4_Yp.txt out4_Y.txt  
cmd n 10 molcount out2.txt  
cmd i 2000 3000 10 molcountsphere Yp 0 -50 230 28 -50 50 -50 50 0 out3_Yp.txt  
cmd i 2000 3000 10 molcountsphere Y 0 -50 230 28 -50 50 -50 50 0 out3_Y.txt  
cmd i 0 3000 1 molcountsphere Yp 0 -50 230 28 -50 50 -50 50 100 out4_Yp.txt  
cmd i 0 3000 1 molcountsphere Y 0 -50 230 28 -50 50 -50 50 100 out4_Y.txt
```

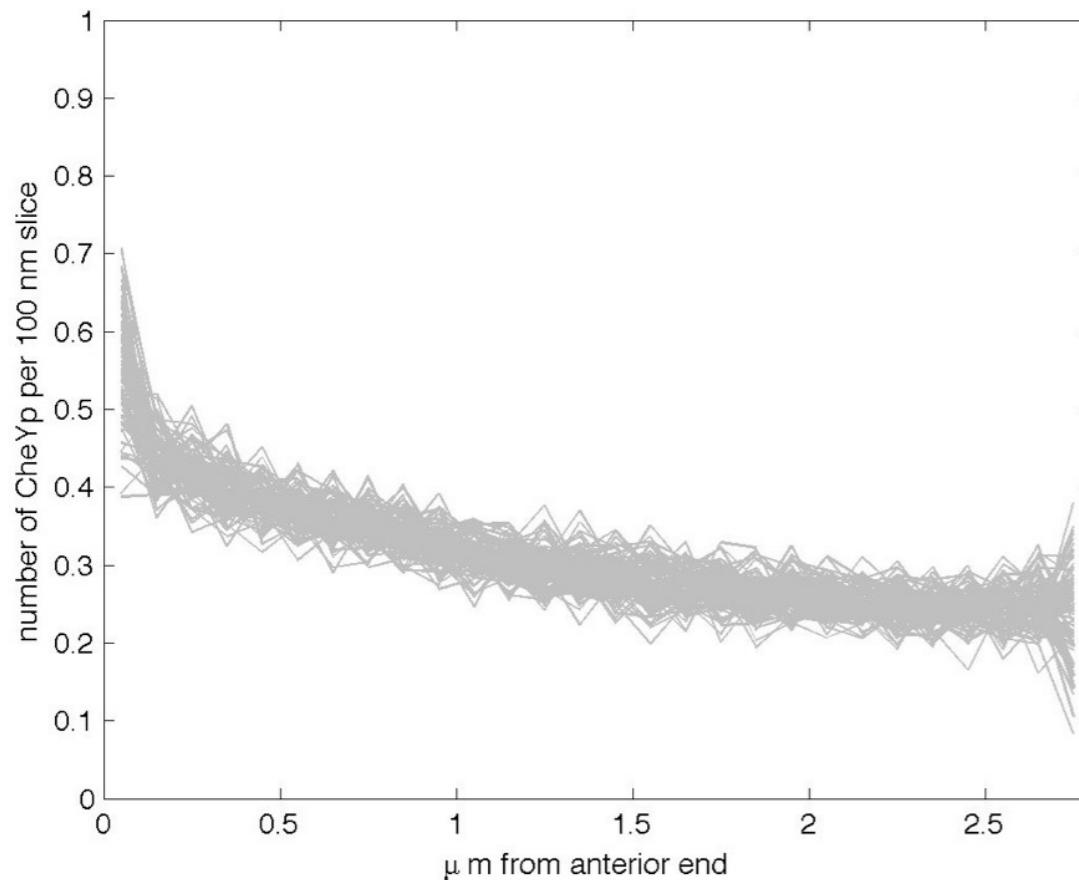
calculate ratio and plot using MATLAB

YprofileRatio.m

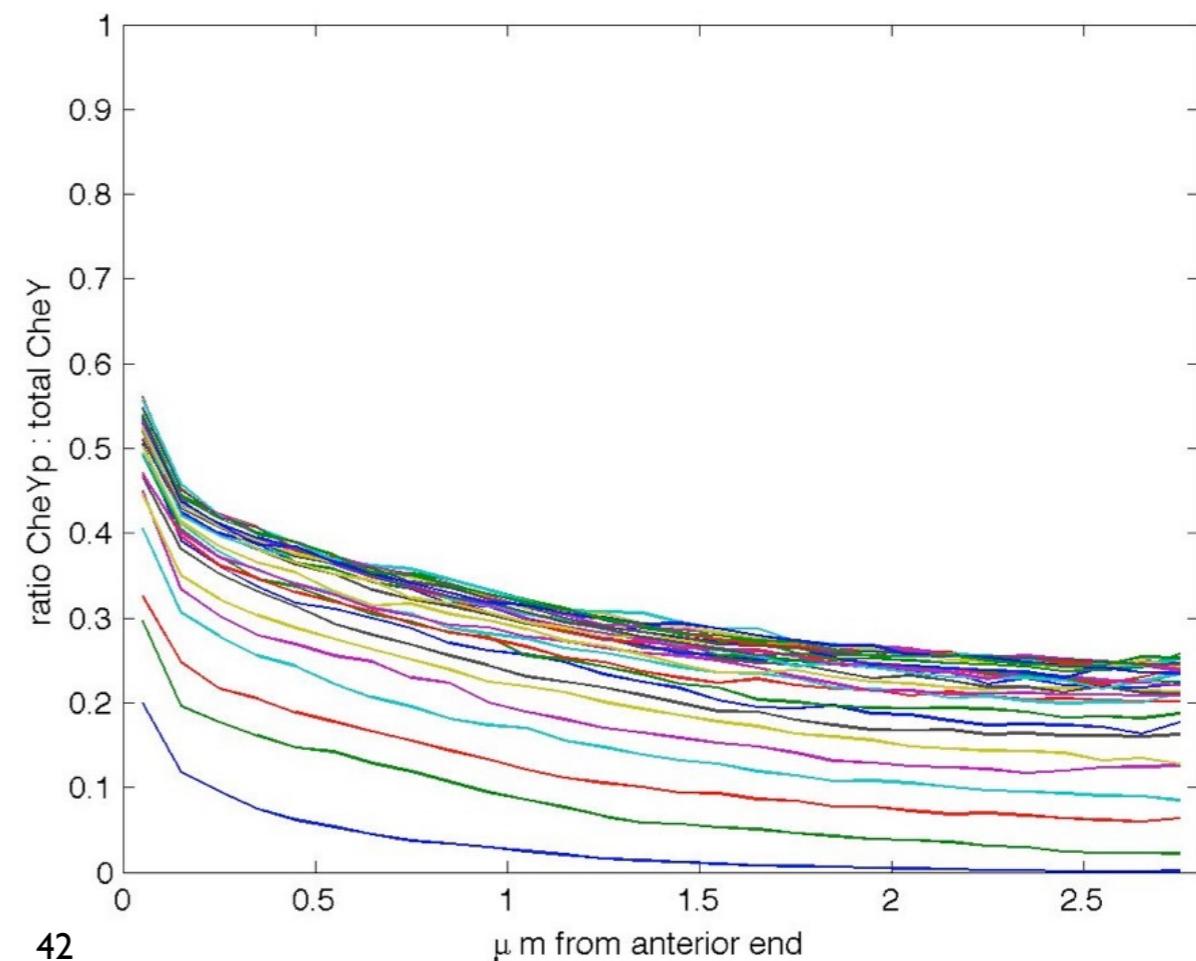
YprofileRatioTime.m

# Spatial distribution

molcountspace (out3\_Y and out3\_Yp) /  
YprofileRatio.m:  
snapshots at steady state (2000-3000 ms)



molcountspace (out4\_Y and out4\_Yp) /  
YprofileRatioTime.m:  
100ms-averages during Yp buildup (0-3000 ms)



# Further things to try with the Smoldyn chemotaxis model

- convert to different units and redo the main simulations
- optimise the simulation speed
- let  $Y$  and  $Y_p$  (or just one of them) diffuse along the inner face of the membrane
- let  $Y$  and/or  $Y_p$  diffuse along a cytoskeletal filament
- add the outer membrane and periplasm
- add transmembrane proteins
- surround the cell by an unbounded-emitter surface (what's that?)
- model small molecules, which can pass through the outer membrane and then bind to proteins in the inner membrane
- model directed transport through the cell membrane
- include macromolecular crowding
- simulate FRAP (fluorescence recovery after photobleaching)