

```
# PAGfp (CaMKIIbeta) diffusion with complete dendrite & spine architecture.
# PSD at spine tip. Actin distributed throughout spine.
# Interaction with cortical actin in dendritic shaft
```

```
graphics opengl
graphic_iter 10
accuracy 1
#tiff_iter 50
#tiff_name movie
```

```
dim 3
names CaMKa CaMKb CaMKc CaMKd NR2B PSDA PSDB A ACMA ACMB
output files data1.txt data2.txt data3.txt data4.txt data5.txt data6.txt data7.txt data8.txt
max_mol 200000
```

```
difc CaMKa 45
difc CaMKb 45
difc CaMKc 45
difc CaMKd 45
difc NR2B 0.0
difc PSDA 0.0
difc PSDB 0.0
difc A 0.0
difc ACMA 0.0
difc ACMB 0.0
```

```
color CaMKa 0.4 0.2 0.1
color CaMKb 0 1 0
color CaMKc 0.4 0.2 0.1
color CaMKd 0 1 0
color NR2B 1 1 0
color PSDA 0.4 0.2 0.1
color PSDB 0 1 0
color A 1 0 0
color ACMA 0.4 0.2 0.1
color ACMB 0 1 0
```

```
background_color 0 0 0
frame_thickness 0
```

```
time_start 0
time_stop 16000
time_step 1
```

```
low_wall 0 -750 r
high_wall 0 750 r
low_wall 1 -750 r
high_wall 1 750 r
low_wall 2 -750 r
high_wall 2 750 r
```

```
# The dendrite is modeled as a rectangle with two bounding plates
```

```
# It runs along the x-axis
mol 3000 CaMKa 250--250 45-35 45-35
mol 3000 CaMKa 250--250 -35--45 -35--45
mol 500 CaMKc 50--50 50--50 -190--100
mol 10 CaMKa 5--5 50--50 50--50
mol 750 NR2B 50--50 50--50 -190--200
```

```
mol 20 A 50 50 -100--200
mol 20 A 50 40 -100--200
mol 20 A 50 30 -100--200
mol 20 A 50 20 -100--200
mol 20 A 50 10 -100--200
mol 20 A 50 0 -100--200
mol 20 A 50 -10 -100--200
mol 20 A 50 -20 -100--200
mol 20 A 50 -30 -100--200
mol 20 A 50 -40 -100--200
mol 20 A 50 -50 -100--200
mol 20 A 40 50 -100--200
mol 20 A 40 40 -100--200
mol 20 A 40 30 -100--200
mol 20 A 40 20 -100--200
mol 20 A 40 10 -100--200
mol 20 A 40 0 -100--200
mol 20 A 40 -10 -100--200
mol 20 A 40 -20 -100--200
```

mol 20 A 40 -30 -100--200
mol 20 A 40 -40 -100--200
mol 20 A 40 -50 -100--200
mol 20 A 30 50 -100--200
mol 20 A 30 40 -100--200
mol 20 A 30 30 -100--200
mol 20 A 30 20 -100--200
mol 20 A 30 10 -100--200
mol 20 A 30 0 -100--200
mol 20 A 30 -10 -100--200
mol 20 A 30 -20 -100--200
mol 20 A 30 -30 -100--200
mol 20 A 30 -40 -100--200
mol 20 A 30 -50 -100--200
mol 20 A 20 50 -100--200
mol 20 A 20 40 -100--200
mol 20 A 20 30 -100--200
mol 20 A 20 20 -100--200
mol 20 A 20 10 -100--200
mol 20 A 20 0 -100--200
mol 20 A 20 -10 -100--200
mol 20 A 20 -20 -100--200
mol 20 A 20 -30 -100--200
mol 20 A 20 -40 -100--200
mol 20 A 20 -50 -100--200
mol 20 A 10 50 -100--200
mol 20 A 10 40 -100--200
mol 20 A 10 30 -100--200
mol 20 A 10 20 -100--200
mol 20 A 10 10 -100--200
mol 20 A 10 0 -100--200
mol 20 A 10 -10 -100--200
mol 20 A 10 -20 -100--200
mol 20 A 10 -30 -100--200
mol 20 A 10 -40 -100--200
mol 20 A 10 -50 -100--200
mol 20 A 0 50 -100--200
mol 20 A 0 40 -100--200
mol 20 A 0 30 -100--200
mol 20 A 0 20 -100--200
mol 20 A 0 10 -100--200
mol 20 A 0 0 -100--200
mol 20 A 0 -10 -100--200
mol 20 A 0 -20 -100--200
mol 20 A 0 -30 -100--200
mol 20 A 0 -40 -100--200
mol 20 A 0 -50 -100--200
mol 20 A -10 50 -100--200
mol 20 A -10 40 -100--200
mol 20 A -10 30 -100--200
mol 20 A -10 20 -100--200
mol 20 A -10 10 -100--200
mol 20 A -10 0 -100--200
mol 20 A -10 -10 -100--200
mol 20 A -10 -20 -100--200
mol 20 A -10 -30 -100--200
mol 20 A -10 -40 -100--200
mol 20 A -10 -50 -100--200
mol 20 A -20 50 -100--200
mol 20 A -20 40 -100--200
mol 20 A -20 30 -100--200
mol 20 A -20 20 -100--200
mol 20 A -20 10 -100--200
mol 20 A -20 0 -100--200
mol 20 A -20 -10 -100--200
mol 20 A -20 -20 -100--200
mol 20 A -20 -30 -100--200
mol 20 A -20 -40 -100--200
mol 20 A -20 -50 -100--200
mol 20 A -30 50 -100--200
mol 20 A -30 40 -100--200
mol 20 A -30 30 -100--200
mol 20 A -30 20 -100--200
mol 20 A -30 10 -100--200
mol 20 A -30 0 -100--200
mol 20 A -30 -10 -100--200
mol 20 A -30 -20 -100--200
mol 20 A -30 -30 -100--200
mol 20 A -30 -40 -100--200
mol 20 A -30 -50 -100--200
mol 20 A -40 50 -100--200

```

mol 20 A -40 40 -100--200
mol 20 A -40 30 -100--200
mol 20 A -40 20 -100--200
mol 20 A -40 10 -100--200
mol 20 A -40 0 -100--200
mol 20 A -40 -10 -100--200
mol 20 A -40 -20 -100--200
mol 20 A -40 -30 -100--200
mol 20 A -40 -40 -100--200
mol 20 A -40 -50 -100--200
mol 20 A -50 50 -100--200
mol 20 A -50 40 -100--200
mol 20 A -50 30 -100--200
mol 20 A -50 20 -100--200
mol 20 A -50 10 -100--200
mol 20 A -50 0 -100--200
mol 20 A -50 -10 -100--200
mol 20 A -50 -20 -100--200
mol 20 A -50 -30 -100--200
mol 20 A -50 -40 -100--200
mol 20 A -50 -50 -100--200

```

```
max_surface 6
```

```
start_surface
```

```

name stalk1
rate CaMKa fsoln front 0.1
rate CaMKa front fsoln 0.001
rate CaMKb fsoln front 0.1
rate CaMKb front fsoln 0.001
color both 0.9 0.4 0.2 0.3
thickness 2
polygon both f
max_panels r 4
panel r -1 250 50 50 -240 -100
panel r -1 250 -50 50 -240 -100
panel r -2 250 50 50 -240 -100
panel r -2 250 50 -50 -240 -100
end_surface

```

```
start_surface
```

```

name stalk2
rate CaMKa fsoln front 0.1
rate CaMKa front fsoln 0.001
rate CaMKb fsoln front 0.1
rate CaMKb front fsoln 0.001
color both 0.9 0.4 0.2 0.3
thickness 2
polygon both f
max_panels r 4
panel r -1 -250 50 50 240 -100
panel r -1 -250 -50 50 240 -100
panel r -2 -250 50 50 240 -100
panel r -2 -250 50 -50 240 -100
end_surface

```

```
start_surface
```

```

name reflectStalk
action both CaMKa r
action both CaMKb a
color both 0.9 0.4 0.2 0.3
thickness 2
polygon both f
max_panels r 2
panel r -0 250 -60 -60 120 120
panel r +0 -250 -60 -60 120 120
end_surface

```

```
start_surface
```

```

name neck
action both all r
color both 0.9 0.4 0.2 0.3
thickness 2
polygon both f
max_panels r 5
panel r -0 20 50 -50 -100 -50
panel r -0 -20 50 -50 -100 -50
panel r -1 20 50 50 -40 -150
panel r -1 20 -50 50 -40 -150
panel r -2 20 50 50 -40 -100

```

end_surface

start_surface

name head

rate CaMKc fsoln front 0.1

rate CaMKc front fsoln 0.001

rate CaMKd fsoln front 0.1

rate CaMKd front fsoln 0.001

color both 0.9 0.4 0.2 0.3

thickness 2

polygon both e

max_panels r 7

panel r -0 50 50 -100 -100 -100

panel r -0 -50 50 -100 -100 -100

panel r -1 50 50 -100 -100 -100

panel r -1 50 -50 -100 -100 -100

panel r -2 50 50 -200 -100 -100

panel r -2 50 50 -100 -30 -100

panel r -2 -50 50 -100 30 -100

end_surface

start_surface

name head-neck

action back CaMKa m

action back CaMKb m

action front CaMKc m

action front CaMKd m

rate CaMKa bsoln fsoln 5 CaMKc

rate CaMKb bsoln fsoln 5 CaMKd

rate CaMKc fsoln bsoln 5 CaMKa

rate CaMKd fsoln bsoln 5 CaMKb

color both 0.9 0.4 0.2 0.3

thickness 2

polygon both f

max_panels r 1

panel r -2 20 50 -100 -40 -100

end_surface

reaction r1 PSDA -> CaMKc + NR2B 1

product_placement r1 pgemmax 0.2

reaction r2 CaMKc + NR2B -> PSDA 100

reaction r3 PSDB -> CaMKd + NR2B 1

product_placement r3 pgemmax 0.2

reaction r4 CaMKd + NR2B -> PSDB 100

reaction r5 ACMA -> CaMKc + A 0.01

product_placement r5 pgemmax 0.2

reaction r6 CaMKc + A -> ACMA 100

reaction r7 ACMB -> CaMKd + A 0.01

product_placement r7 pgemmax 0.2

reaction r8 CaMKd + A -> ACMB 100

cmd b keypress u

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#cmd i 0 6000 1 excludebox -40 40 -40 40 -155 -125

#cmd i 0 6000 1 excludebox -250 250 -15 15 -30 30

cmd @ 6000 replacevolmol CaMKa CaMKb -50 50 -50 50 -50 50

cmd i 0 16000 50 listmols3 CaMKa data1.txt

cmd i 0 16000 50 listmols3 CaMKc data2.txt

cmd i 0 16000 50 listmols3 CaMKb data3.txt

cmd i 0 16000 50 listmols3 CaMKd data4.txt

```
cmd i 0 16000 50 listmols3 PSDA data5.txt  
cmd i 0 16000 50 listmols3 PSDB data6.txt  
cmd i 0 16000 50 listmols3 ACMA data7.txt  
cmd i 0 16000 50 listmols3 ACMB data8.txt
```

```
end_file
```