# Smoldyn

**What it is.** Smoldyn is a computer program for cell-scale biochemical simulations. It simulates each molecule of interest individually to capture stochasticity and yield nanometer-scale spatial resolution. Simulated molecules diffuse, react, and interact with surfaces in realistic ways. Most parts were written by and are maintained by Steve Andrews.

**Installation.** First, download Smoldyn package from http://www.smoldyn.org.

Mac: Open your Terminal application for command line access. In download directory, enter `sudo ./install.sh`, and follow prompts. See README.txt file.

Windows: Get a command prompt with Start/All programs/Accessories/Command prompt. The executable is smoldyn.exe and necessary dll files should be in the Windows directory.

Linux: Build from source using CMake.

**Example file**

```
# Enzymatic reactions on a surface, by Steve Andrews, October 2009.
# This model is in the public domain.  Units are microns and seconds.
```
comments with author, date, availablility and units

```
define K_FWD 0.001
define K_BACK 1
define K_PROD 1
```
define statements for text replacement. Helps keep parameters together.

```
dim 2
boundaries 0 -1 1
boundaries 1 -1 1
time_start 0
time_stop 10
time_step 0.01
```
system dimensionality (1 to 3), outer boundaries, and simulation time

```
species S E ES P
difc S 3
difc P 3
color S(all) green
color E(all) darkred
color ES(all) orange
color P(all) darkblue
display_size all(all) 0.02
display_size E(all) 0.03
display_size ES(all) 0.03
```
list of species (S = substrate, E = enzyme, ES = complex, P = product)
other species information, with diffusion coefficients, color, display size, etc.
Can also list drift velocity or anisotropic diffusion matrix.

```
graphics opengl_good
frame_thickness 0
```
graphics quality, and system drawing instructions

```
start_surface membrane
  action both all reflect
  color both black
  thickness 1
  panel sphere 0 0 1 50
end_surface
```
block with surface name and definition. action gives molecule behavior upon contact with front and back surface faces. rate gives adsorption, desorption, and transmission rate. List surface panels and graphics attributes.

```
reaction fwd E(front) + S(bsoln) -> ES(front) K_FWD
reaction back ES(front) -> E(front) + S(bsoln) K_BACK
product_placement back pgemmax 0.2
reaction prod ES(front) -> E(front) + P(bsoln) K_PROD
```
reaction list with reactions and reaction rates.
product_placement is for reversible reactions.

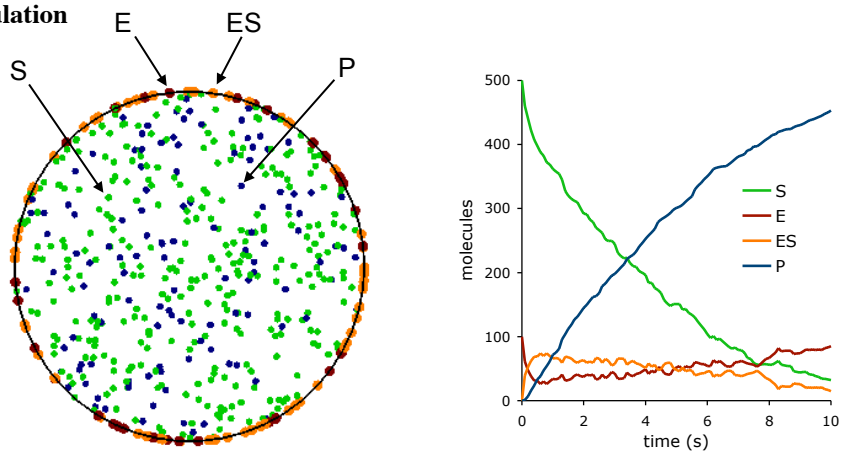
```
start_compartment inside
  surface membrane
  point 0 0
end_compartment
```
block with compartment name and definition. A compartment is defined by bounding surfaces and one or more “interior-defining points”

```
compartment_mol 500 S inside
surface_mol 100 E(front) membrane all all
```
molecule placements for starting condition

```
text_display time S E(front) ES(front) P
output_files MMBexampleout.txt
cmd B molcountheader MMBexampleout.txt
cmd N 10 molcount MMBexampleout.txt
```
simulation output. text_display is to graphics window and rest is to MMBexampleout.txt file for post-processing.

```
end_file
```
end of the simulation file

**Output of example simulation**




**Runtime flags.** Entered on command line.

| flag | result |
|---|---|
| | normal: parameters displayed and simulation run |
| -o | suppress output: text output files are not opened |
| -p | parameters only: simulation is not run |
| -q | quiet: parameters are not displayed |
| -t | text only: no graphics are displayed |
| -V | display version number and quit |
| -v | verbose: extra parameter information is displayed |
| -w | suppress warnings: no warnings are shown |

**Graphics manipulations.** Graphics window must be active.

| Key | function |
|---|---|
| space | toggle pause mode between on and off |
| Q | quit |
| T | save image as TIFF file |
| 0 | reset view to default |
| arrows | rotate object |
| shift, arrows | pan object |
| = | zoom in |
| - | zoom out |
| x,y,z | rotate counterclockwise about object axis |
| X,Y,Z | rotate clockwise about object axis |

**Units.** Smoldyn does not assume any units, so the user needs to keep units consistent within each simulation.

| | Concentration | Diffusion coefficient | Unimolec. reactions | Bimolecular reactions | Adsorption rates |
|---|---|---|---|---|---|
| Typical | 10 μM | 10 $\mu m^2 s^{-1}$ | 1 $s^{-1}$ | $10^5$ $M^{-1} s^{-1}$ | 1 μm $s^{-1}$ |
| mks | $6x10^{21}$ $m^{-3}$ | $10^{-11}$ $m^2 s^{-1}$ | 1 $s^{-1}$ | $10^2$ $m^3 mol^{-1} s^{-1}$<br>$1.7x10^{-22}$ $m^3 s^{-1}$ | $10^{-6}$ m $s^{-1}$ |
| cgs | $6x10^{15}$ $cm^{-3}$ | $10^{-7}$ $cm^2 s^{-1}$ | 1 $s^{-1}$ | $1.7x10^{-16}$ $cm^3 s^{-1}$ | $10^{-4}$ cm $s^{-1}$ |
| μm-ms | 6000 $\mu m^{-3}$ | $10^{-2}$ $\mu m^2 ms^{-1}$ | $10^{-3}$ $ms^{-1}$ | $1.7x10^{-7}$ $\mu m^3 ms^{-1}$ | $10^{-3}$ μm $ms^{-1}$ |
| μm-s | 6000 $\mu m^{-3}$ | 10 $\mu m^2 s^{-1}$ | 1 $s^{-1}$ | $1.7x10^{-4}$ $\mu m^3 s^{-1}$ | 1 μm $s^{-1}$ |
| nm-ms | $6x10^{-6}$ $nm^{-3}$ | $10^4$ $nm^2 ms^{-1}$ | $10^{-3}$ $ms^{-1}$ | 170 $nm^3 ms^{-1}$ | 1 nm $ms^{-1}$ |
| nm-μs | $6x10^{-6}$ $nm^{-3}$ | 10 $nm^2 \mu s^{-1}$ | $10^{-6}$ $\mu s^{-1}$ | 0.17 $nm^3 \mu s^{-1}$ | $10^{-3}$ nm $\mu s^{-1}$ |

**Colors.** Enter with color name or with red, green, blue color coordinates, each ranging from 0 to 1.

maroon olive royal darkred red green sky darkorange scarlet chartreuse aquamarine darkyellow rose khaki violet darkgreen brick purple mauve darkblue pink magenta orchid darkviolet brown fuchsia plum lightred tan lime azure lightorange sienna teal black lightyellow orange aqua gray lightgreen salmon cyan grey lightblue coral blue silver lightviolet yellow navy slate gold turquoise white

**Command timing.** Commands are used for system output or for system manipulation.

| integer queue | |
|---|---|
| B | once, before simulation starts |
| A | once, after simulation ends |
| @ *i* | once, at iteration *i* |
| I *on off dt* | every *dti* iteration, from ≥ *oni* to ≤ *offi* |
| E | every time step |
| N *n* | every *n* time steps |

| continuous time queue | |
|---|---|
| b | once, before simulation starts |
| a | once, after simulation ends |
| @ *time* | once, at ≥ *time* |
| i *on off dt* | every *dt*, from ≥ *on* until ≤ *off* |
| x *on off dt xt* | geometric progression |

**Surface panel shapes.** rectangle, triangle, sphere, hemisphere, cylinder, disk

**Publications about Smoldyn**

Andrews and Bray, *Phys. Biol.* 1:137, 2004; Andrews, *Phys. Biol.* 2:111, 2005; Andrews, *Phys. Biol.* 6:046015, 2009; Andrews et al. *PLoS Comp. Biol.* 6:e1000705, 2010; Andrews, *Meth. in Mol. Biol.* 804:519, 2012.