MMBioS

Introduction to Microphysiological Simulations Using MCell

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MCell is a Monte Carlo reaction-diffusion simulator for modeling cellular microphysiology in arbitrarily complex 3D spatial geometries.
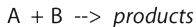
Computational Microphysiology: The simulation of biological systems at micron to millimeter length scales (subcellular to cellular) using realistic 3D geometries over biological timescales from *ns* to *ms* to *s*.
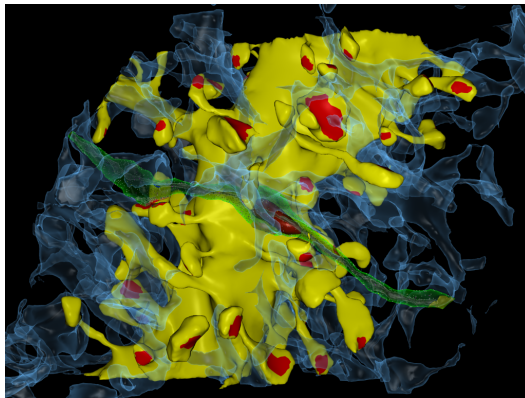
1. Realistic 3D Geometry
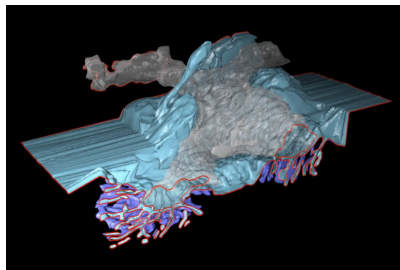
2. Random Walk Diffusion

A + B --> *products*
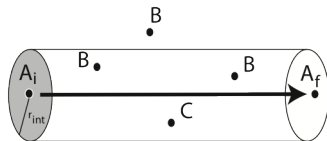
3. Stochastic Biochemical State Transition
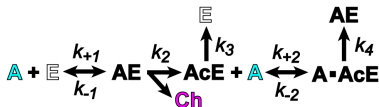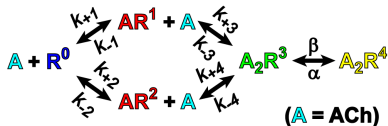
(A = ACh)

Obtain or Create Model Mesh Geometry

↓

Annotate Meshes

↓

Specify Non-Spatial Model Parameters

↓

Simulate Model

↓

Visualize and Analyze Results

Model geometries for MCell simulations can be obtained via:

1. Reconstruction of model mesh geometry from electron microscopy data

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2. Generative models of cell organization from fluorescence microscopy imaging (**Day 3**)
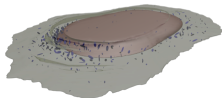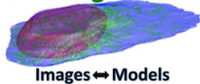
Model geometries for MCell simulations can be obtained via:

1. Reconstruction of model mesh geometry from electron microscopy data
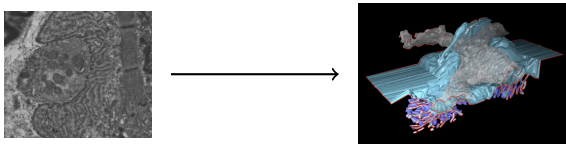
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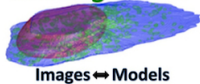
3. *In silico* geometry construction based on average geometry
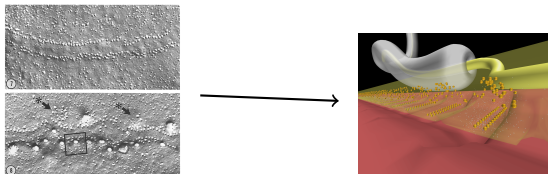
Show 24 active zone model
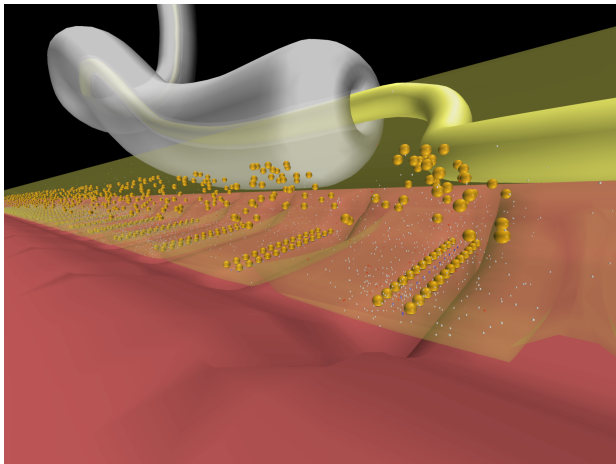
Obtain or Create Model Mesh Geometry
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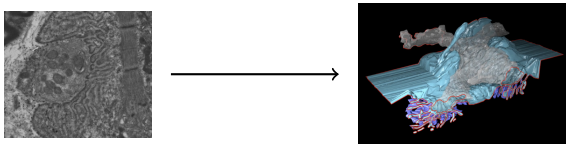Visualize and Analyze Results

Beyond a geometry specification, MCell models typically also contain

- **Molecules**: can diffuse in space (volume molecules) or on mesh surfaces (surface molecules); need diffusion coefficients, concentrations/densities, locations.

- **Reactions**: requires knowledge of all elementary reaction pathways (uni and bimolecular) and the corresponding reaction rate constants.
  Complex reaction networks can be described using rule based approaches via **BioNetGen** and then be imported into MCell models via CellBlender (**Day 2**).

- **Output Specification**: request output for visualisation and analysis purposes; may require definition of additional geometry objects such as counting or sampling boxes.
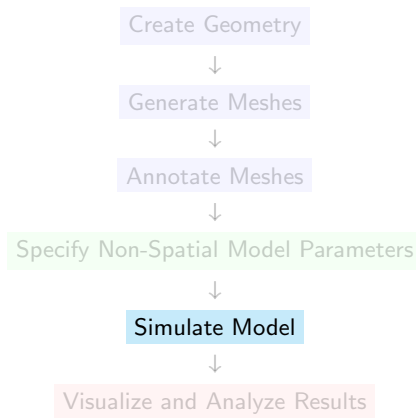
Create Geometry

↓

Generate Meshes

↓

Annotate Meshes

↓

Specify Non-Spatial Model Parameters

↓

Simulate Model

↓

Visualize and Analyze Results

MCell simulations are run on the command line or from within CellBlender.

```
# mcell my_model.mdl
```

my_model.mdl contains the complete model description as Model Description Language (MDL).

Simulate Your Model

MCell simulations are run on the command line or from within CellBlender.

```
# mcell my_model.mdl
```

my_model.mdl contains the complete model description as Model Description Language (MDL).

```
# mcell -seed 10 my_model.mdl
```

Create Geometry

↓

Generate Meshes

↓

Annotate Meshes

↓

Specify Non-Spatial Model Parameters

↓

Simulate Model

↓

Visualize and Analyze Results
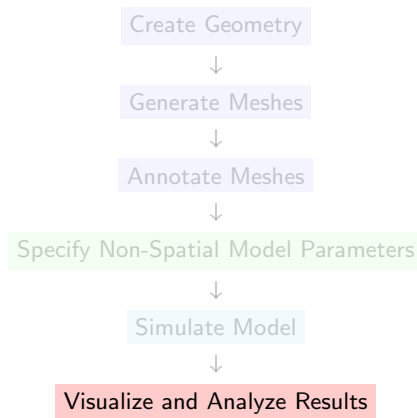
MCell can produce two types of output (you specify how much of each, what molecules, etc.):

- Visualization Output for viewing via CellBlender, contains the specification of geometric meshes and the location and orientation of surface and volume molecules.
- Reaction data output, contains time series of
  - volume molecules counts in specified regions of the model
  - surface molecule counts on specified regions of the model
  - reaction counts
  - hits or crossings of surface regions by volume molecules
  - ...

  Reaction data can be plotted with CellBlender and also be analyzed using external tools, e.g. `R`, `python`, `octave`, `MATLAB`, etc..
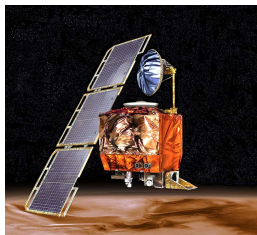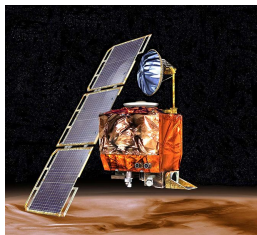
Mars Climate Orbiter, September 23, 1999
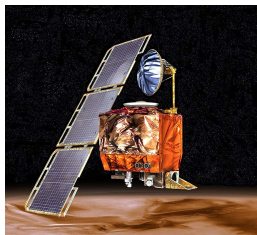
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```
The MCO MIB has determined that the root cause for the loss
of the MCO spacecraft was the failure to use metric units in
the coding of a ground software file [...] The output from
the SM_FORCES application code as required by a MSOP Project
Software Interface Specification (SIS) was to be in metric
units of Newtonseconds (N-s). Instead, the data was reported
in English units of pound-seconds (lbf-s). [...] An erroneous
trajectory was computed using this incorrect data.
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Don't let your MCell model become the next MCO!

- Spatial dimensions are in units of microns (μm, $10^{-6} m$).
- Time is in units of seconds.
- Diffusion coefficients are in units of $cm^2 s^{-1}$.
- Uni-molecular reaction rate constants are in s^{-1}.
- Bi-molecular reaction rate constants between two volume or a volume and surface molecule are in $Mol^{-1} s^{-1}$.
- Bi-molecular reaction rate constants between two surface molecules are in $\mu m^2 \#^{-1} s^{-1}$.
- Each simulation runs for a specified number of iterations.
- The duration of an iteration is one timestep.

MCell models are described using Model Description Language (MDL) (see
`http://www.mcell.org/documentation/mcell3_qrg.xhtml`
for a comprehensive list of keywords.)

MDL commands are written in ALL CAPS and consist of

- simple statements of the form

```
MDL_COMMAND = <value>
```

- statement blocks enclosed in curly braces describing a certain aspect of the
  simulation (geometry and release object definition, molecule definition)

```
MDL_BLOCK { <block content> }
```

where `<block content>` are other `MDL_COMMAND`s or `MDL_BLOCK`s.

Your First Model - Simulation Prologue

Each MCell simulation needs to define the simulation *timestep* (TIME_STEP) and the number of *iterations* (ITERATIONS).

first_model.mdl

```
/* define variables for timestep
   and iterations */
iters = 100
dt   = 1e-6

/* use variable to set actual keywords */
ITERATIONS = iters
TIME_STEP = dt
```

Notes:

- Within MDL you can define arbitrary variables (such as iters, dt).
- MDL is case sensitive - do not use ALL_CAPS for variables to avoid clashes with MCell keywords.
- You can use C-style comments (/* */ and single line //).

Next, we use CellBlender to construct a mesh which defines the 3D geometry of our model. We create a simple cube shaped object and export it in MDL format, `Cube.mdl`.
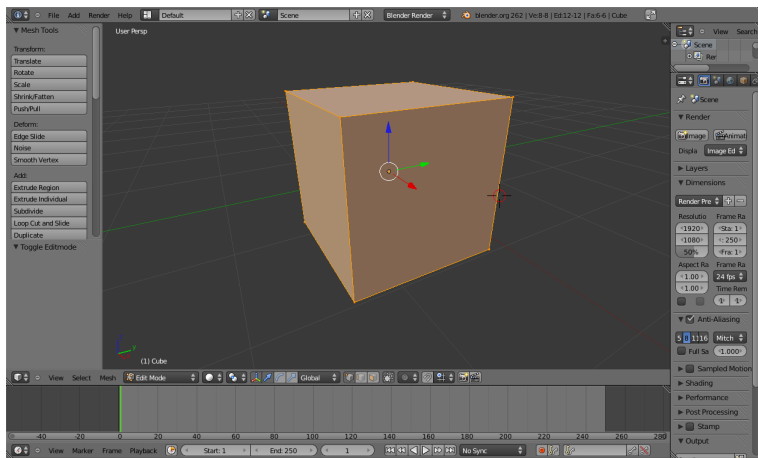
Then we add `Cube.mdl` to our MDL file ....

first_model.mdl

```
iters = 100
dt    = 1e-6
ITERATIONS = iters
TIME_STEP = dt

INCLUDE_FILE = "./Cube.mdl"
```

Notes:

- MDL files can include other MDL files which is very useful for organizing them, e.g., according to model component (geometry description, molecule definitions, etc.).
- Inclusion is lexical and thus the order of `INCLUDE` statements does matter.

Cube.mdl

```
Cube POLYGON_LIST
{
  VERTEX_LIST
  {
    [ 1, 0.999999940395355, -1 ]
    [ 1, -1, -1 ]
    [ -1.00000011920929, -0.999999821186066, -1 ]
    [ -0.999999642372131, 1.00000035762787, -1 ]
    [ 1.00000047683716, 0.999999463558197, 1 ]
    [ 0.999999344348907, -1.00000059604645, 1 ]
    [ -1.00000035762787, -0.999999642372131, 1 ]
    [ -0.999999940395355, 1, 1 ]
  }
  ELEMENT_CONNECTIONS
  {
    [ 4, 0, 3 ]
    [ 4, 3, 7 ]
    [ 2, 6, 7 ]
    [ 2, 7, 3 ]
    [ 1, 5, 2 ]
    [ 5, 6, 2 ]
    [ 0, 4, 1 ]
    [ 4, 5, 1 ]
    [ 4, 7, 5 ]
    [ 7, 6, 5 ]
    [ 0, 1, 2 ]
    [ 0, 2, 3 ]
  }
  DEFINE_SURFACE_REGIONS
  {
    top
    {
      ELEMENT_LIST = [8, 9]
    }
  }
}
```

Cube.mdl

```
Cube POLYGON_LIST
{
  VERTEX_LIST
  {
    [ 1, 0.999999940395355, -1 ]
    [ 1, -1, -1 ]
    [ -1.00000011920929, -0.999999821186066, -1 ]
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    [ 1.00000047683716, 0.999999463558197, 1 ]
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    [ -1.00000035762787, -0.999999642372131, 1 ]
    [ -0.999999940395355, 1, 1 ]
  }
  ELEMENT_CONNECTIONS
  {
    [ 4, 0, 3 ]
    [ 4, 3, 7 ]
    [ 2, 6, 7 ]
    [ 2, 7, 3 ]
    [ 1, 5, 2 ]
    [ 5, 6, 2 ]
    [ 0, 4, 1 ]
    [ 4, 5, 1 ]
    [ 4, 7, 5 ]
    [ 7, 6, 5 ]
    [ 0, 1, 2 ]
    [ 0, 2, 3 ]
  }
  DEFINE_SURFACE_REGIONS
  {
    top
    {
      ELEMENT_LIST = [8, 9]
    }
  }
}
```

Notes:

- Our Cube object is a `POLYGON_LIST` object, the most general way of specifying a geometrical shape within MDL.

- MCell also provides geometric primitives to define object geometry and molecule `RELEASE_SITE`s.

- `DEFINE_SURFACE_REGIONS` allows one to group subsets of triangles into surface regions.

- Meshes are by default reflective to all diffusing volume molecules but can be made absorptive or transparent via *surface classes*.

… and then make it part of the actual simulation model by adding it to the INSTANTIATEed main object.

first_model.mdl

```
iters = 100
dt    = 1e-6
ITERATIONS = iters
TIME_STEP = dt

INCLUDE_FILE = "./Cube.mdl"

INSTANTIATE World OBJECT {
  Cube OBJECT Cube{}
}
```

first_model.mdl

```
...

INCLUDE_FILE = "./Cube.mdl"

INSTANTIATE World OBJECT {
  Cube OBJECT Cube{}
}

...
```

Notes:

- Geometry objects can be combined into "meta" objects (here a single one called `World`).
- Within meta objects new geometry objects can be created, or exisiting objects can be copied and transformed (translation, rotation, scaling).
- Meta objects can be nested, i.e. contain other meta objects.

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Molecules are defined within a `DEFINE_MOLECULES` block. Our cube model will contain two volume molecules `Vol1`, `Vol2` and a surface molecule `Surf`.

first_model.mdl

```
iters = 100
dt    = 1e-6
ITERATIONS = iters
TIME_STEP = dt

DEFINE_MOLECULES {
  Vol1 {DIFFUSION_CONSTANT_3D = 1E-6}
  Vol2 {DIFFUSION_CONSTANT_3D = 1E-6}
  Surf  {DIFFUSION_CONSTANT_2D = 1E-7}
}

INCLUDE_FILE = "./Cube.mdl"

INSTANTIATE World OBJECT {
  Cube OBJECT Cube{}
}
```

Notes:

- Volume and surface molecules are distinguished via providing either a 3D or 2D diffusion coefficient.
- the units of the diffusion coefficient are $cm^2 s^{-1}$
- molecules in MCell are point particles

Your First Model - Adding Molecules

Up to this point we only **defined** the molecules in our simulation but we haven't **released** any!

first_model.mdl

```
...

DEFINE_MOLECULES {
  Vol1 {DIFFUSION_CONSTANT_3D = 1E-6}
  Vol2 {DIFFUSION_CONSTANT_3D = 1E-6}
  Surf {DIFFUSION_CONSTANT_2D = 1E-7}
}

INCLUDE_FILE = "./Cube.mdl"

INSTANTIATE World OBJECT {
  Cube OBJECT Cube{}

  vol1_rel RELEASE_SITE {
      SHAPE = World.Cube
      MOLECULE = Vol1
      NUMBER_TO_RELEASE = 2000
  }
  surf1_rel RELEASE_SITE {
      SHAPE = World.Cube[top]
      MOLECULE = Surf'
      NUMBER_TO_RELEASE = 2000
  }

}
```

- Volume and surface molecules can be released within RELEASE_SITE blocks.

Up to this point we only **defined** the molecules in our simulation but we haven't **released** any!

first_model.mdl

```
...

DEFINE_MOLECULES {
  Vol1 {DIFFUSION_CONSTANT_3D = 1E-6}
  Vol2 {DIFFUSION_CONSTANT_3D = 1E-6}
  Surf {DIFFUSION_CONSTANT_2D = 1E-7}
}

INCLUDE_FILE = "./Cube.mdl"

INSTANTIATE World OBJECT {
  Cube OBJECT Cube{}

  vol1_rel RELEASE_SITE {
      SHAPE = World.Cube
      MOLECULE = Vol1
      NUMBER_TO_RELEASE = 2000
  }
  surf1_rel RELEASE_SITE {
      SHAPE = World.Cube[top]
      MOLECULE = Surf'
      NUMBER_TO_RELEASE = 2000
  }

}
```

- Volume and surface molecules can be released within RELEASE_SITE blocks.
- For volume molecules the SHAPE keyword needs to reference a **closed** geometry object (qualified starting from the instantiated top level object) in which to release the molecules.

Your First Model - Adding Molecules

Up to this point we only **defined** the molecules in our simulation but we haven't **released** any!

```
first_model.mdl
...

DEFINE_MOLECULES {
  Vol1 {DIFFUSION_CONSTANT_3D = 1E-6}
  Vol2 {DIFFUSION_CONSTANT_3D = 1E-6}
  Surf {DIFFUSION_CONSTANT_2D = 1E-7}
}

INCLUDE_FILE = "./Cube.mdl"

INSTANTIATE World OBJECT {
  Cube OBJECT Cube{}

  vol1_rel RELEASE_SITE {
      SHAPE = World.Cube
      MOLECULE = Vol1
      NUMBER_TO_RELEASE = 2000
  }
  surf1_rel RELEASE_SITE {
      SHAPE = World.Cube[top]
      MOLECULE = Surf'
      NUMBER_TO_RELEASE = 2000
  }
}

}
```

- Volume and surface molecules can be released within `RELEASE_SITE` blocks.
- For volume molecules the `SHAPE` keyword needs to reference a **closed** geometry object (qualified starting from the instantiated top level object) in which to release the molecules.
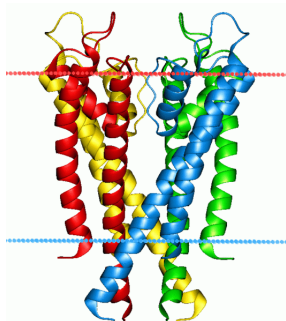- For surface molecules the `SHAPE` keyword defines a surface region on a geometry object (here `top` on `World.Cube` via the `GeometryObject[<region specifier>]` syntax).
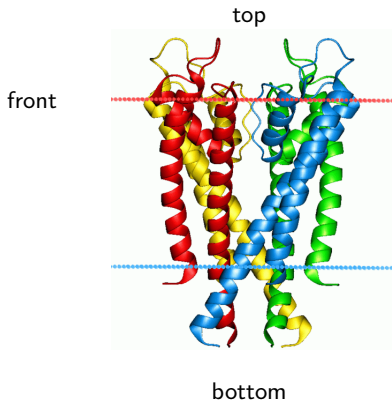
KcsA (image from Wikipedia)
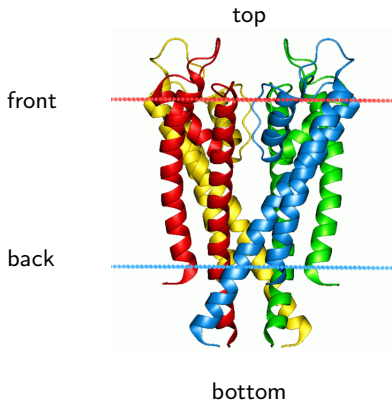
top

KcsA (image from Wikipedia)

top

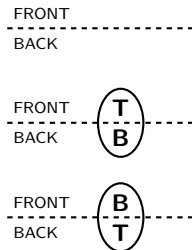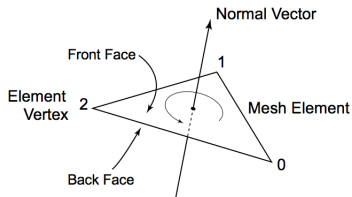bottom

KcsA (image from Wikipedia)

- Surface molecules have a **top** and **bottom** domain.

top

front

bottom

KcsA (image from Wikipedia)

- Surface molecules have a **top** and **bottom** domain.

top

front

back

bottom

KcsA (image from Wikipedia)

- Surface molecules have a **top** and **bottom** domain.
- Surfaces (membranes) have a **front** and **back**.

How does MCell handle surface molecule orientation?

- mesh tiles and thus surfaces have a unique front and back according to the *right hand rule*.
  Note: Your mesh tiles need to have a consisted orientation!
- surface molecules are either placed with their top at the front or the back of the surface!
- each mesh element is subdivided into (triangular) tiles which can each accommodate only a single surface molecules; surface molecules "acquire" a certain surface area. The tile density can be set via `SURFACE_GRID_DENSITY` (default $10000 \ \mu m^{-2}$).
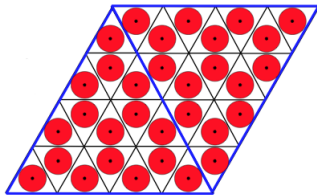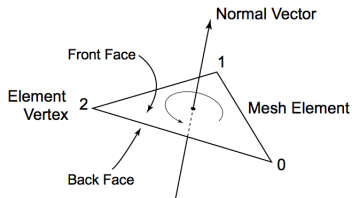
How does MCell handle surface molecule orientation?

- mesh tiles and thus surfaces have a unique front and back according to the *right hand rule*.
  Note: Your mesh tiles need to have a consisted orientation!
- surface molecules are either placed with their top at the front or the back of the surface!
- each mesh element is subdivided into (triangular) tiles which can each accommodate only a single surface molecules; surface molecules "acquire" a certain surface area. The tile density can be set via `SURFACE_GRID_DENSITY` (default 10000 μm^{-2}).

Now we can understand MCell's surface molecule placement syntax.

first_model.mdl

```
...

surf1_rel RELEASE_SITE {
   SHAPE = World.Cube[top]
   MOLECULE = Surf'
   NUMBER_TO_RELEASE = 2000
}
...
```

- **Surf'** places the molecule with its top at the FRONT of the surface.

Now we can understand MCell's surface molecule placement syntax.

first_model.mdl
```
...

surf1_rel RELEASE_SITE {
  SHAPE = World.Cube[top]
  MOLECULE = Surf'
  NUMBER_TO_RELEASE = 2000
}
...
```

- `Surf'` places the molecule with its top at the FRONT of the surface.

- `Surf,` places the molecule with its top at the BACK of the surface.

Now we can understand MCell's surface molecule placement syntax.

first_model.mdl

```
...

surf1_rel RELEASE_SITE {
  SHAPE = World.Cube[top]
  MOLECULE = Surf'
  NUMBER_TO_RELEASE = 2000
}
...
```

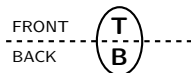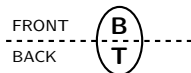- `Surf'` places the molecule with its top at the FRONT of the surface.

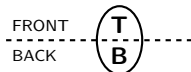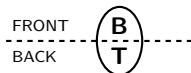- `Surf,` places the molecule with its top at the BACK of the surface.

- `Surf;` places the molecule with its top randomly at the FRONT or BACK of the surface.
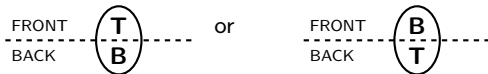
Now that we have defined molecules and placed them in the `World` we can define reactions between them.

first_model.mdl

```
...

DEFINE_MOLECULES {
  Vol1 {DIFFUSION_CONSTANT_3D = 1E-6}
  Vol2 {DIFFUSION_CONSTANT_3D = 1E-6}
  Surf {DIFFUSION_CONSTANT_2D = 1E-7}
}

DEFINE_REACTIONS {
  /* creation of Vol2 */
  Vol1        -> Vol2 [1e4]

  /* annihilation of Vol2 */
  Vol2 + Vol2 -> NULL [1e6] : annih

  /* transport of Vol1 across surface
   * via Surf */
  Vol1, + Surf' -> Vol1' + Surf' [1e7]
}
```

- The general reaction syntax is

  `reactant(s) -> product(s) [rate] : name`

- Reactions can be named and then counted.

Now that we have defined molecules and placed them in the `World` we can define reactions between them.

first_model.mdl

```
...

DEFINE_MOLECULES {
  Vol1 {DIFFUSION_CONSTANT_3D = 1E-6}
  Vol2 {DIFFUSION_CONSTANT_3D = 1E-6}
  Surf {DIFFUSION_CONSTANT_2D = 1E-7}
}

DEFINE_REACTIONS {
  /* creation of Vol2 */
  Vol1      -> Vol2 [1e4]

  /* annihilation of Vol2 */
  Vol2 + Vol2 -> NULL [1e6] : annih

  /* transport of Vol1 across surface
   * via Surf */
  Vol1, + Surf' -> Vol1' + Surf' [1e7]
}
```

- The general reaction syntax is

  `reactant(s) -> product(s) [rate] : name`

- Reactions can be named and then counted.
- The units are
  - $[s^{-1}]$ for unimolecular reactions,
  - $[M^{-1}s^{-1}]$ for bimolecular reactions between two volume or a volume and a surface molecule.
  - $[\mu m^2 \#^{-1} s^{-1}]$ for bimolecular reactions between two surface molecules.
- Make sure your simulation parameters are such that reaction probabilities remain < 1.

Now that we have defined molecules and placed them in the `World` we can define reactions between them.

```
first_model.mdl
 ...

 DEFINE_MOLECULES {
   Vol1 {DIFFUSION_CONSTANT_3D = 1E-6}
   Vol2 {DIFFUSION_CONSTANT_3D = 1E-6}
   Surf {DIFFUSION_CONSTANT_2D = 1E-7}
 }

 DEFINE_REACTIONS {
   /* creation of Vol2 */
   Vol1       -> Vol2 [1e4]

   /* annihilation of Vol2 */
   Vol2 + Vol2 -> NULL [1e6] : annih

   /* transport of Vol1 across surface
    * via Surf */
   Vol1, + Surf' -> Vol1' + Surf' [1e7]
 }
```

- The general reaction syntax is

  `reactant(s) -> product(s) [rate] : name`

- Reactions can be named and then counted.
- The units are
  - $[s^{-1}]$ for unimolecular reactions,
  - $[M^{-1}s^{-1}]$ for bimolecular reactions between two volume or a volume and a surface molecule.
  - $[\mu m^2 \#^{-1} s^{-1}]$ for bimolecular reactions between two surface molecules.
- Make sure your simulation parameters are such that reaction probabilities remain < 1.

What is going on in the reaction involving `Vol1` and `Surf`?

How do we properly write reactions involving surface molecules in MCell?

```
first_model.mdl
  ...

  DEFINE_REACTIONS
    /* creation of Vol2 */
    Vol1       -> Vol2 [1e4]

    /* annihilation of Vol2 */
    Vol2 + Vol2 -> NULL [1e6] : annih

    /* transport of Vol1 across surface
     * via Surf */
    Vol1, + Surf' -> Vol1' + Surf' [1e7]
```

- Any reaction involving surface molecules requires orientation specifiers for **each** molecular player (volume and surface) involved.
- The *relative* location of orientation specifiers determines the relative orientation molecules need to have in order for the reaction to proceed.

How do we properly write reactions involving surface molecules in MCell?

first_model.mdl

```
...

DEFINE_REACTIONS
  /* creation of Vol2 */
  Vol1        -> Vol2 [1e4]

  /* annihilation of Vol2 */
  Vol2 + Vol2 -> NULL [1e6] : annihi

  /* transport of Vol1 across surface
   * via Surf */
  Vol1, + Surf' -> Vol1' + Surf' [1e7]
```

Since `Vol1` and `Surf` have

- opposite specifiers on the reactant side, `Vol1` reacts with the **bottom** of `Surf`.
- matching specifiers on the product side, `Vol1` reacts with the **top** of `Surf`.

How do we properly write reactions involving surface molecules in MCell?

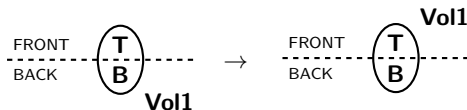### first_model.mdl

```
...

DEFINE_REACTIONS
  /* creation of Vol2 */
  Vol1      -> Vol2 [1e4]

  /* annihilation of Vol2 */
  Vol2 + Vol2 -> NULL [1e6] : annihi

  /* transport of Vol1 across surface
   * via Surf */
  Vol1, + Surf' -> Vol1' + Surf' [1e7]
```

Since `Vol1` and `Surf` have

- opposite specifiers on the reactant side, `Vol1` reacts with the **bottom** of `Surf`.
- matching specifiers on the product side, `Vol1` reacts with the **top** of `Surf`.

Your First Model - Reactions Involving Surface Molecules

How do we properly write reactions involving surface molecules in MCell?

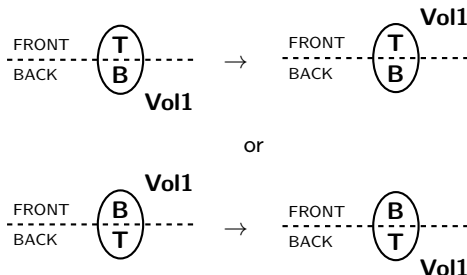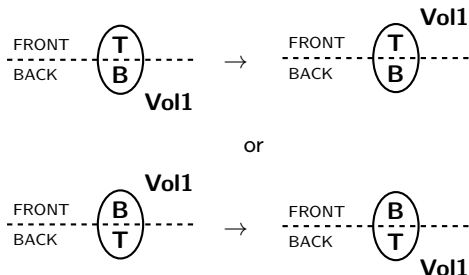### first_model.mdl

```
...

DEFINE_REACTIONS
  /* creation of Vol2 */
  Vol1       -> Vol2 [1e4]

  /* annihilation of Vol2 */
  Vol2 + Vol2 -> NULL [1e6] : annihi

  /* transport of Vol1 across surface
   * via Surf */
  Vol1, + Surf' -> Vol1' + Surf' [1e7]
```
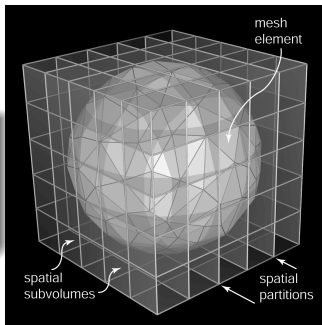
Since Vol1 and Surf have

- opposite specifiers on the reactant side, Vol1 reacts with the **bottom** of Surf.
- matching specifiers on the product side, Vol1 reacts with the **top** of Surf.

We will learn more about surface reactions later!

first_model.mdl

```
   ...
PARTITION_X = [[-1.0 TO 1.0 STEP 0.1]]
PARTITION_Y = [[-1.0 TO 1.0 STEP 0.1]]
PARTITION_Z = [[-1.0 TO 1.0 STEP 0.1]]
   ...
```

- Partitioning into spatial subvolumes is used by MCell to significantly speed up simulations via *divide and conquer*.

first_model.mdl

```
  ...
PARTITION_X = [[-1.0 TO 1.0 STEP 0.1]]
PARTITION_Y = [[-1.0 TO 1.0 STEP 0.1]]
PARTITION_Z = [[-1.0 TO 1.0 STEP 0.1]]
  ...
```

- Partitioning into spatial subvolumes is used by MCell to significantly speed up simulations via *divide and conquer*.
- Especially for larger models experimenting to find the proper partitioning scheme can lead to significant simulation speedup.
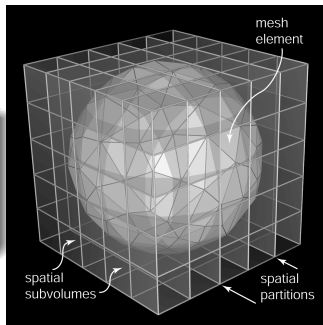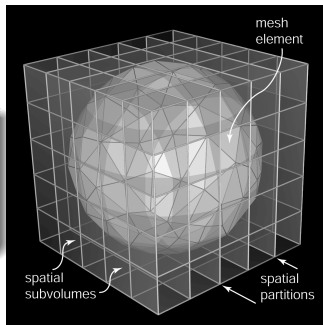
first_model.mdl

```
  ...
PARTITION_X = [[-1.0 TO 1.0 STEP 0.1]]
PARTITION_Y = [[-1.0 TO 1.0 STEP 0.1]]
PARTITION_Z = [[-1.0 TO 1.0 STEP 0.1]]
  ...
```

- Partitioning into spatial subvolumes is used by MCell to significantly speed up simulations via *divide and conquer*.
- Especially for larger models experimenting to find the proper partitioning scheme can lead to significant simulation speedup.
- Good partitioning requires hand tuning.
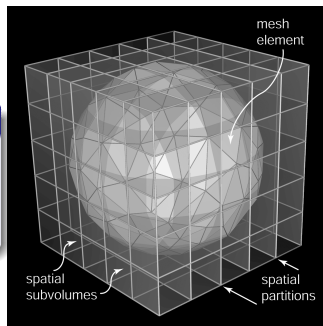
first_model.mdl

```
  ...
PARTITION_X = [[-1.0 TO 1.0 STEP 0.1]]
PARTITION_Y = [[-1.0 TO 1.0 STEP 0.1]]
PARTITION_Z = [[-1.0 TO 1.0 STEP 0.1]]
  ...
```

- Partitioning into spatial subvolumes is used by MCell to significantly speed up simulations via *divide and conquer*.
- Especially for larger models experimenting to find the proper partitioning scheme can lead to significant simulation speedup.
- Good partitioning requires hand tuning.
- There is a "sweet spot" between speed up due to an increased number of spatial subvolumes and excessive memory consumption.

MCell provides to types of output

- Visualization Output for viewing your simulation in CellBlender.
- Reaction Data Output provides counts of molecules, events, reactions etc. in plain text ASCII format for further processing in your favourite tool.

first_model.mdl

```
iters = 100
dt    = 1e-6
ITERATIONS = iters
TIME_STEP = dt

cubeVolume = 1e-15
Na = 6.02214129e23

...

INSTANTIATE World OBJECT {
  Cube OBJECT Cube {}
  ...
}

REACTION_DATA_OUTPUT {
  STEP = dt
  {(COUNT[Vol1,WORLD])/cubeVolume/Na}
    => "./react_data/vol1_conc.dat"

  {COUNT[Vol2,WORLD]}
    => "./react_data/vol2.dat"
}
```

- Reaction data output is requested via a `REACTION_DATA_OUTPUT` block.
- `STEP` defines the interval at which to produce output.
- `COUNT` statements define what events to count and output. The general syntax is

```
{COUNT[name , WORLD]} => "<filename>"     or
{COUNT[name , object]} => "<filename>"    or
{COUNT[name , region]} => "<filename>"
```

where `name` is the name of a molecule or reaction.
- Output is typically in two column format

```
      ...
     time1   count1
     time2   count2
     time3   count3
      ...
```

Your First Model - Visualization Data Output

first_model.mdl

```
iters = 100
dt = 1e-6
ITERATIONS = iters
TIME_STEP  = dt
...

VIZ_OUTPUT {
  VIZ_MOLECULE_FORMAT = CELLBLENDER
  FILENAME = "viz_data"
  MOLECULES {
      NAME_LIST {ALL_MOLECULES}
      ITERATION_NUMBERS {ALL_DATA @ ALL_ITERATIONS}
  }
}
```

- Visualization data output is requested via a `VIZ_OUTPUT` block.
- `VIZ_MOLECULE_FORMAT` defines the format of output the output and should be `CELLBLENDER` for compatibility with CellBlender.
- `FILENAME` defines the name of the master viz header file.
- `NAME_LIST` is a whitespace separated list of molecule names to output. `ALL_MOLECULES` outputs all molecules.
- `ITERATION_NUMBERS` defines what to output (`POSITIONS`, `ORIENTATIONS` or `ALL_DATA`) and when to output as a list of iterations (or `ALL_ITERATIONS`)

Visualization data can be read and visualized by CellBlender.