2. Single Molecule Diffusion

2.1. Required software

This tutorial is designed for Blender 2.74, CellBlender 1.0, and MCell 3.3.

> **Note:** Other versions may work as well.

2.2. Tutorial Overview

This tutorial will define a single molecule and show its diffusion.

2.3. Initial Configuration

Install MCell, Blender, and CellBlender if you haven't already done so. Then complete the *First Time Running CellBlender* tutorial and return here.

> **Note:** Alternatively, if you have used CellBlender and Blender before, but you want to start with a "clean slate", try the *Start with a Clean Slate* tutorial.

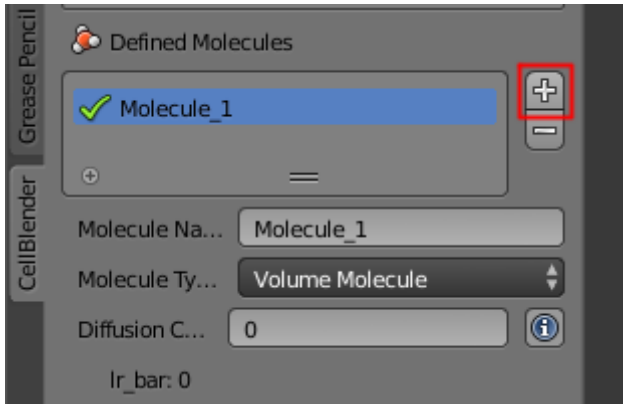
2.3.1. Save the File with a New Name in Your Working Directory

- Start Blender
- Select **File** > **Save As...**
- Change **untitled.blend** to **single_molecule.blend**
- Click **Save As Blender File** button

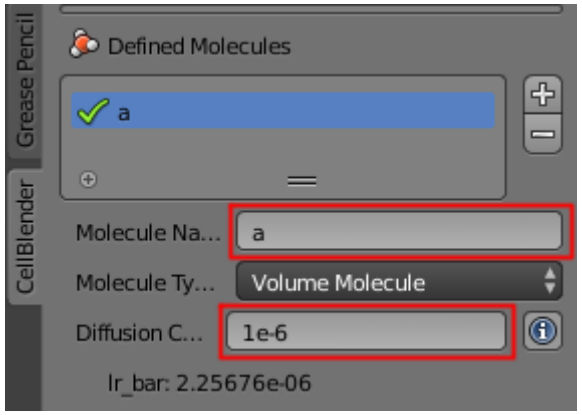
2.3.2. Define a Molecule "species"

- Click the **Molecules** button

- Click the "plus" sign (**+**) to the right of the **Defined Molecules** box



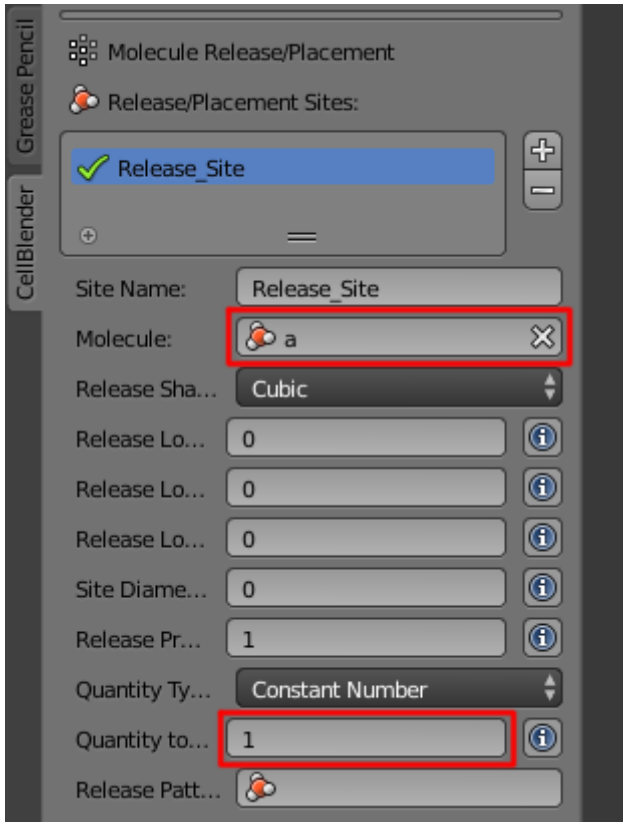
- Click in the **Molecule Name** field, type the letter **a** and press the Enter key
- The new molecule **a** should have a green check mark in the **Defined Molecules** box
- Click in the **Diffusion Constant** box, type **1e-6** and press the Enter key



2.3.3. Release a Single Molecule into the Simulation

- Click the **Molecule Placement** button

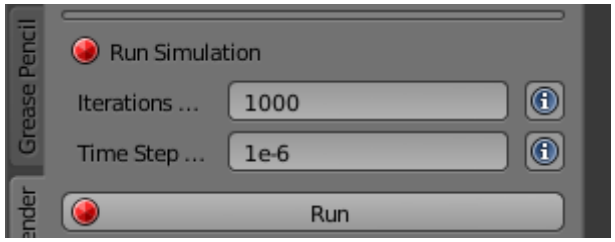
- Click the "plus" sign (**+**) to the right of the **Release/Placement Sites** box
- Click in the **Molecule** field and select the **a** molecules
- Click in the **Quantity to Release** field and set it to **1**



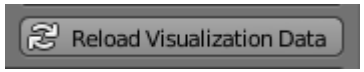
2.3.4. Simulate the Model

- Click the **Run Simulation** button

- Click the **Run** button



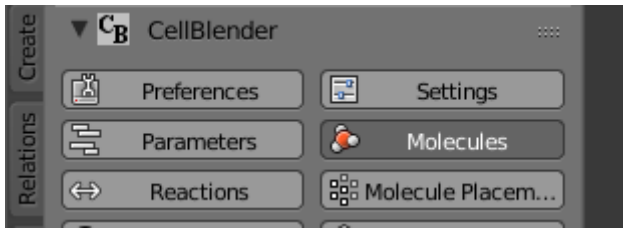
- A green check mark will appear in the list of **MCell Processes** when the simulation is complete
- Press the **Reload Visualization Data** button to load the results of the simulation



2.3.5. Change Settings to See Results

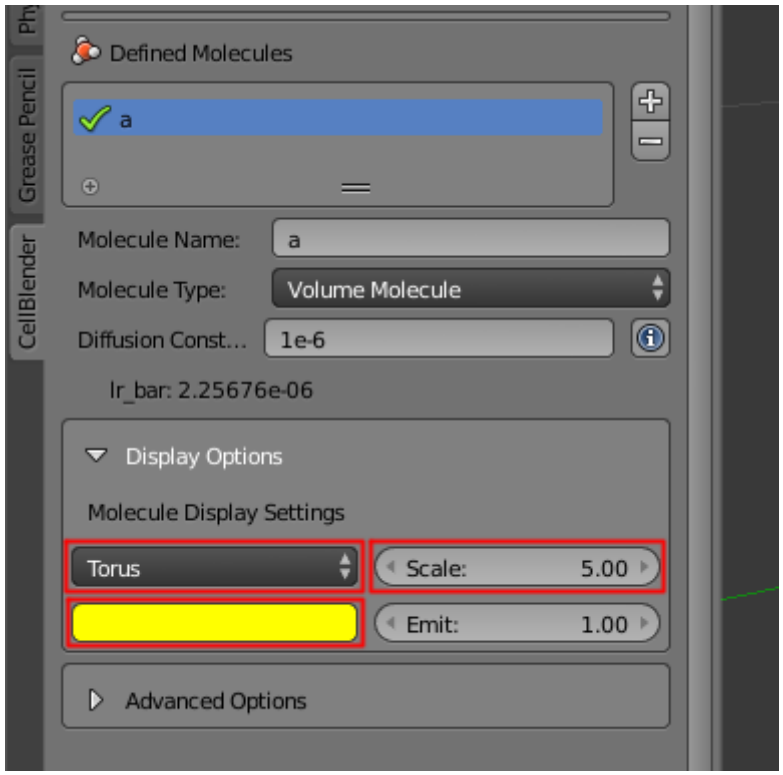
- Hide the "Manipulator" near the bottom middle of the screen

- Click the **Molecules** button



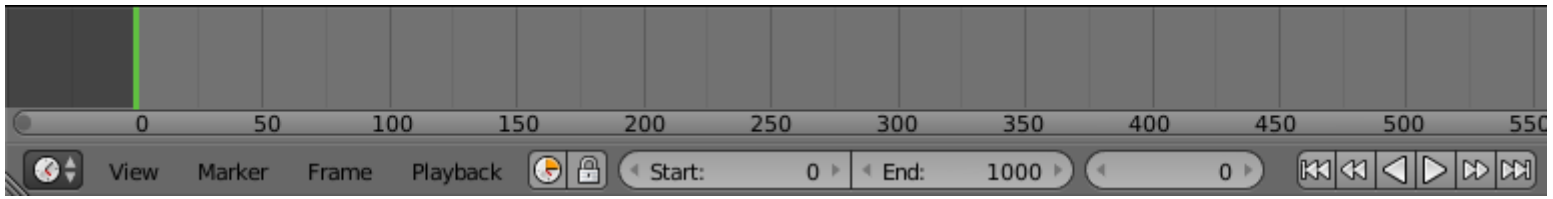
- Open the **Display Options** subpanel

- Change the **Cone** to **Torus**
- Change the **Scale** to **5**
- Change the color to a bright yellow

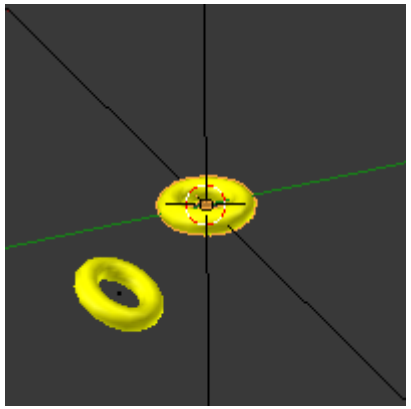


Note: You'll notice that there are actually two torus objects. One of them should be moving as the simulation is played, and the other should be stationary at the origin. The torus at the origin is really a "template" molecule used by Blender. There will always be a template molecule at the origin for every molecule species you define.

2.3.6. Use the Time Line



- Press the "Play" () button below the time line
- Use the scroll wheel to zoom in until you can see the moving torus



- Stop the simulation by clicking the "Pause" () button below the time line
- Click at various locations on the time line to see the molecule state at that time
- Click and drag in the time line to "scrub" the simulation through time

2.3.7. Save Your File

- **File** > **Save**

3. Unimolecular Reactions

3.1. Tutorial Overview

This tutorial will define a single unimolecular reaction.

3.2. Initial Configuration

This tutorial builds upon what was done in *Single Molecule Diffusion*. Either complete that tutorial yourself or use the single_molecule.blend file to get started.

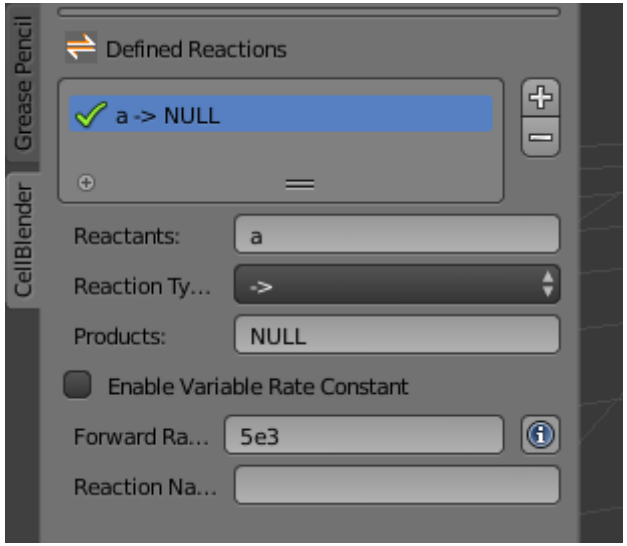
3.2.1. Save the File with a New Name in Your Working Directory

- Select **File** > **Save As...**
- Change **single_molecule.blend** to **unimol_reactions.blend**
- Click **Save As Blender File** button

3.2.2. Define a Reaction

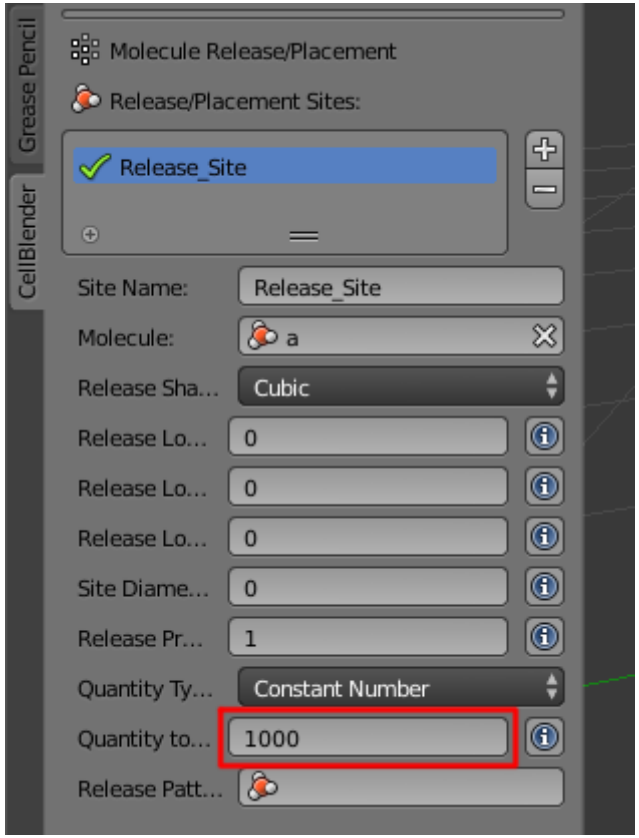
- Click the **Reactions** button.

- Click the "plus" sign (**+**) to the right of the **Defined Reactions** box
- Type **a** in the **Reactants** text field
- Type **NULL** in the **Products** text field
- Type **5e3** in the **Forward Rates** text field



3.2.3. Release More Molecules

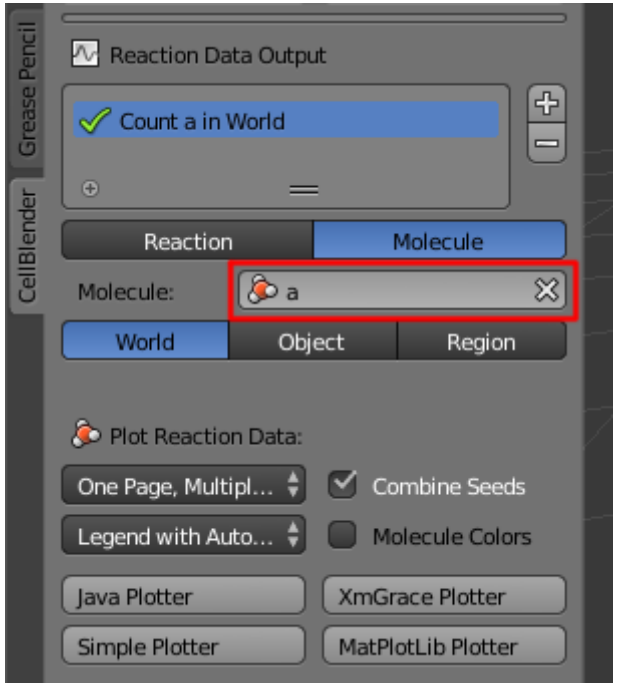
- Click the **Molecule Placement** button
- Change the **Quantity to Release** to **1000**



3.2.4. Create Reaction Data

- Click the **Plot Output Settings** button

- Click the "plus" sign (**+**) to the right of the **Reaction Data Output** box
- Select **a** from the **Molecule** selector.



3.2.5. Simulate the Model

- Click the **Run Simulation** button

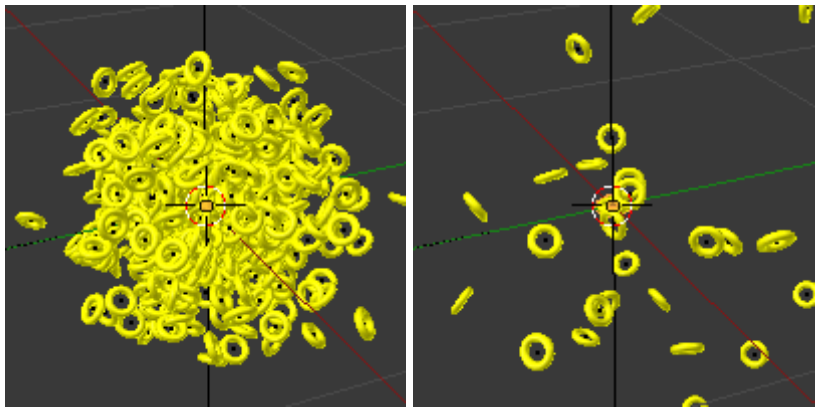
- Click the **Run** button

- Wait for the simulation to complete

- Press the "Reload Visualization Data" button to load the results of the simulation.

3.2.6. Use the Time Line

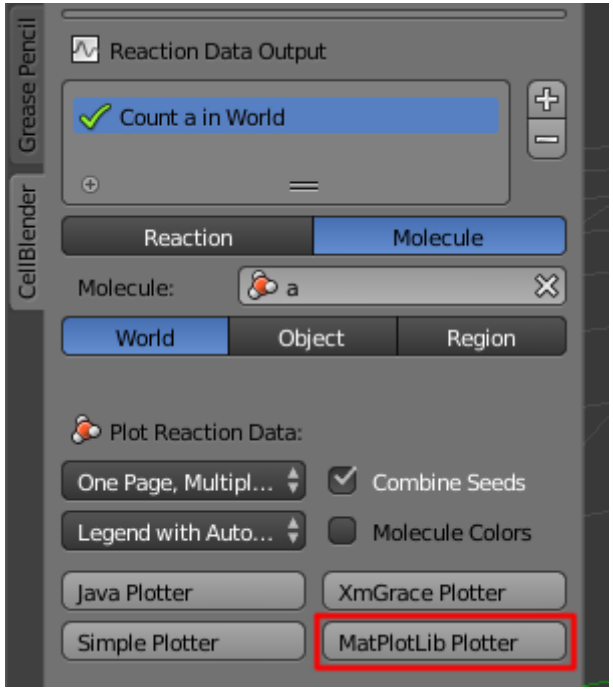
- Press the "Play" () button below the time line

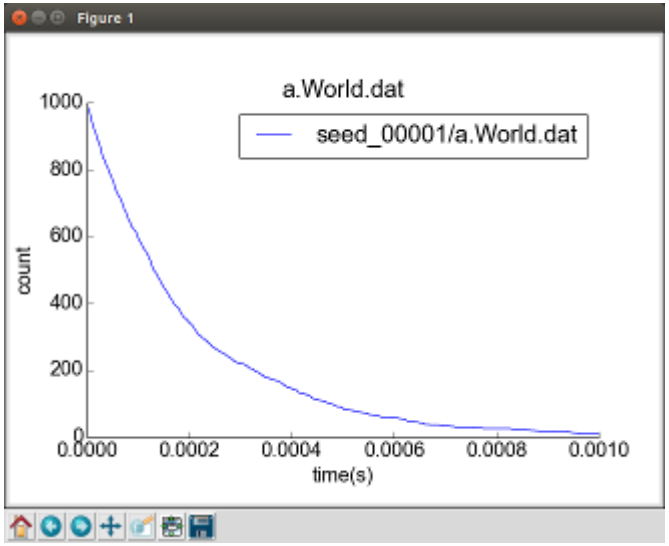


- Stop the simulation by clicking the "Pause" () button below the time line

3.2.7. Plot the Reaction Data

- Click the **Plot Output Settings** button
- Click the **MatPlotLib Plotter** button if it's available.





3.2.8. Save Your File

- **File** > **Save**

4. Add Simple Mesh Geometry

4.1. Tutorial Overview

In this tutorial, a sphere will be added to the simulation around the diffusing molecules.

4.2. Initial Configuration

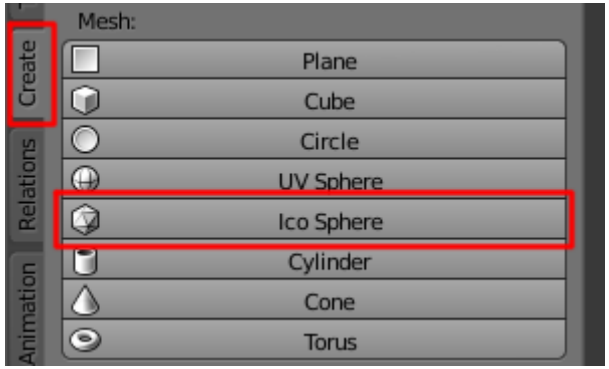
This tutorial builds upon what was done in *Unimolecular Reactions*. Either complete that tutorial yourself or use the unimol_reactions.blend file to get started.

4.2.1. Save the File with a New Name in Your Working Directory

- Select **File** > **Save As...**
- Change **unimol_reactions.blend** to **add_meshgeom.blend**
- Click **Save As Blender File** button

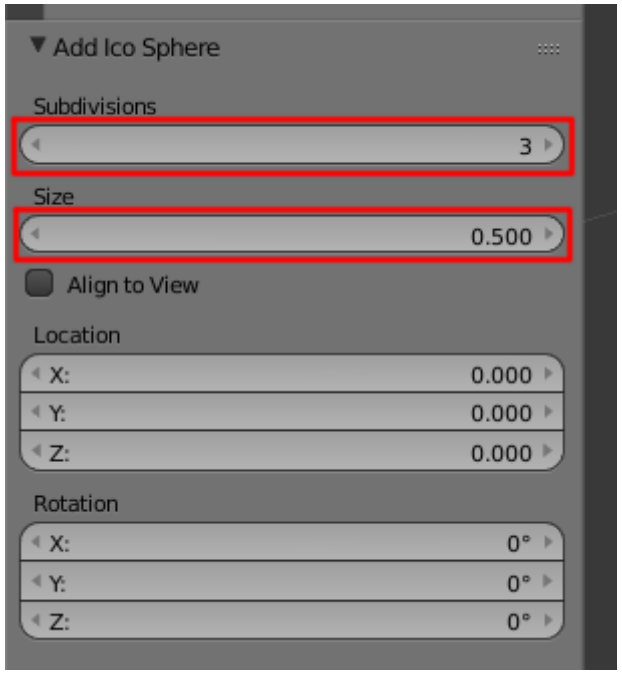
4.2.2. Add Sphere

- Click the **Create** tab
- Hit the **Ico Sphere** button



- The **Add Ico Sphere** options appear in the lower left corner
- Change **Subdivisions** to **3**

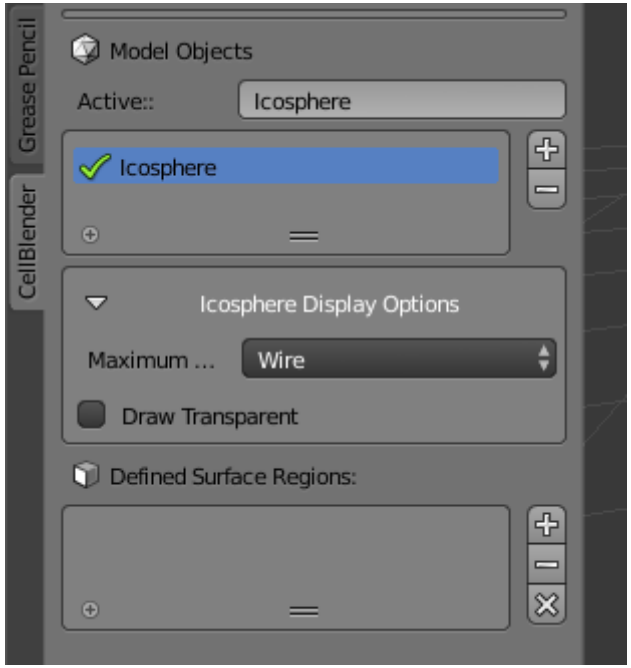
- Change **Size** to **0.5**
- Change each **Location** (**X**, **Y**, and **Z**) to **0.0** if it isn't set already.



4.2.3. Add Sphere to Model Objects

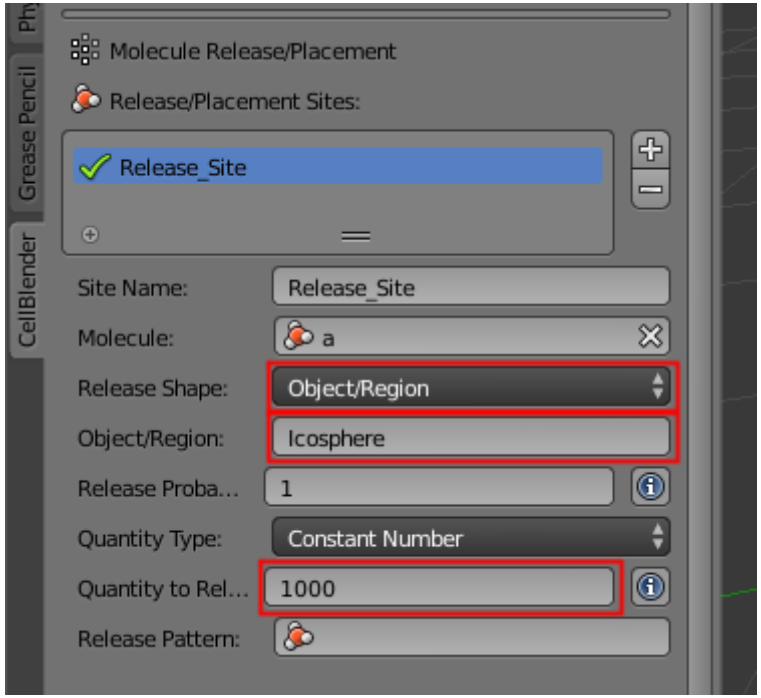
- Click the **CellBlender** tab
- Click the **Model Objects** button

- Click the "plus" sign (**+**) to the right of the **Model Objects** box
- Expand the **Icosphere Display Options** panel
- Change **Maximum Draw Type** to **Wire**



4.2.4. Release Molecules inside Sphere

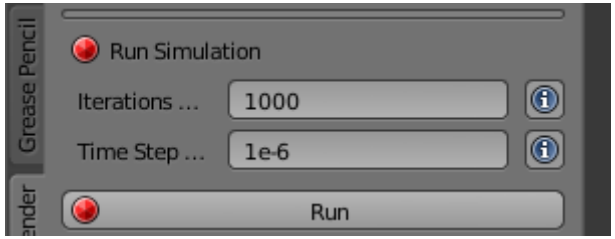
- Click the **Molecule Placement** button
- Select **Release_Site**
- Change **Release Shape** to **Object/Region**
- Type **Icosphere** in the **Object/Region** field
- Change **Quantity to Release** to **1000**



4.2.5. Simulate the Model

- Click the **Run Simulation** button

- Click the **Run** button

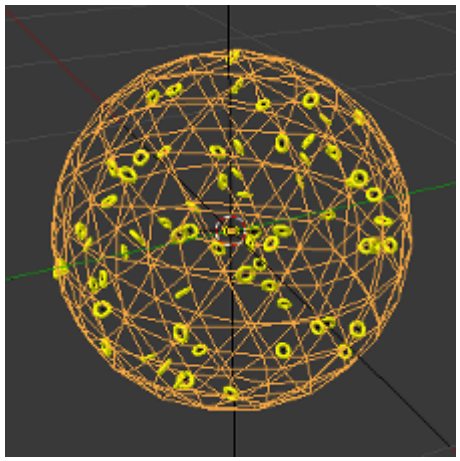


- Wait for the simulation to complete

- Press the "Reload Visualization Data" button to load the results of the simulation.

4.2.6. View the Results

- Press the "Play" () button below the time line



4.2.7. Save Your File

- **File** > **Save**

5. Bimolecular Reactions

5.1. Tutorial Overview

This tutorial will define a single bimolecular reaction.

5.2. Initial Configuration

This tutorial builds upon what was done in *Add Simple Mesh Geometry*. Either complete that tutorial yourself or use the add_meshgeom.blend file to get started.

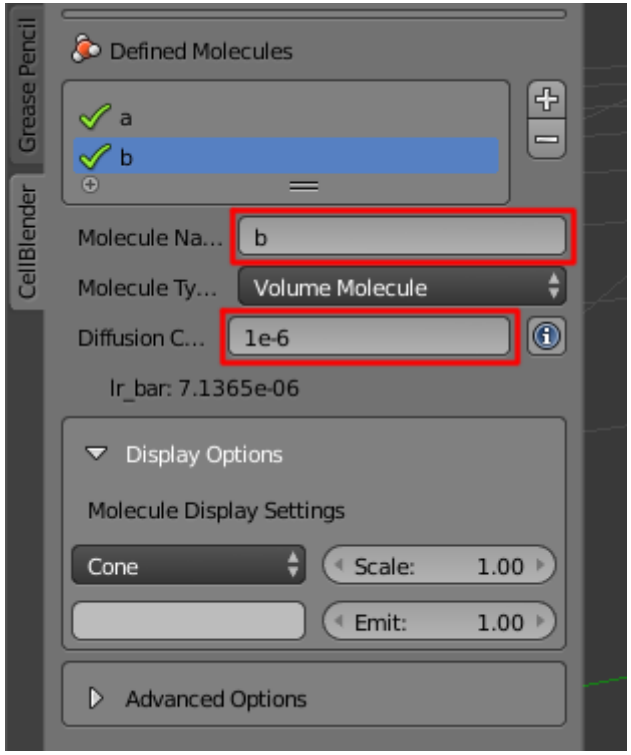
5.2.1. Save the File with a New Name in Your Working Directory

- Select **File** > **Save As...**
- Change **add_meshgeom.blend** to **bimol_reactions.blend**
- Click **Save As Blender File** button

5.2.2. Define a New Molecule Type

- Click the **Molecules** button

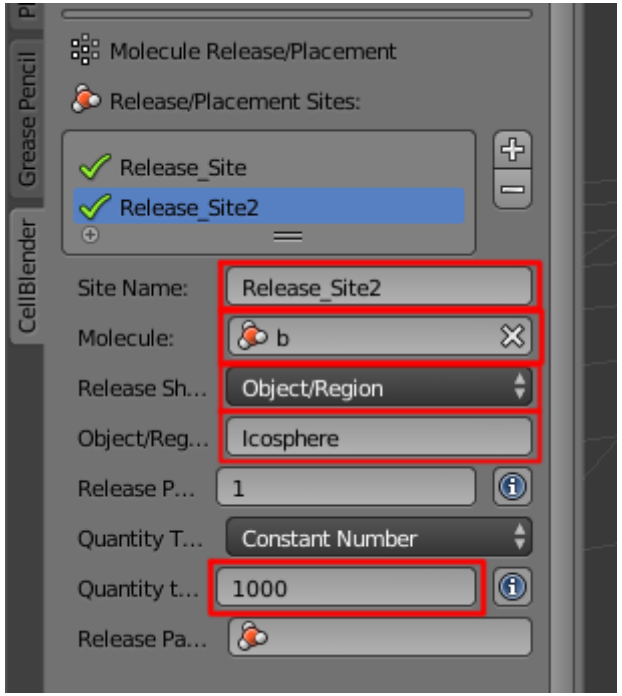
- Click the "plus" sign (**+**) to the right of the **Defined Molecules** box
- Click in the **Molecule Name** field, type the letter **b** and press the Enter key
- Click in the **Diffusion Constant** box, type **1e-6** and press the Enter key



5.2.3. Release "b" Molecules into the Simulation

- Click the **Molecule Placement** button

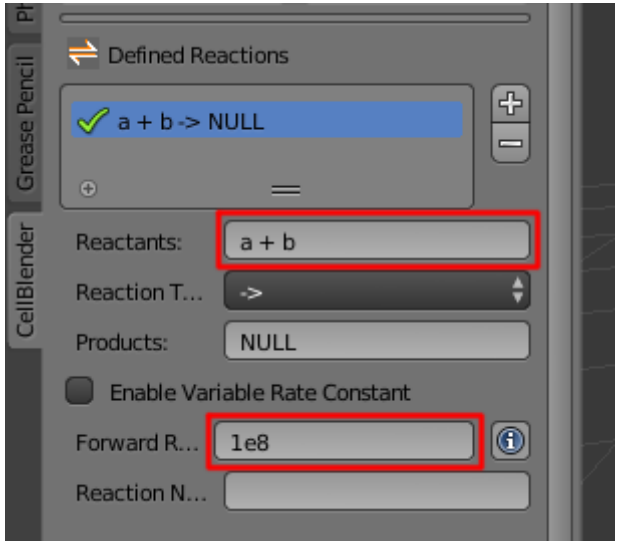
- Click the "plus" sign (**+**) to the right of the **Release/Placement Sites** box
- Change the **Site Name** to **Release_Site2**
- Click in the **Molecule** field and select the **b** molecules
- Change **Release Shape** to **Object/Region**
- Type **Icosphere** in the **Object/Region** field
- Click in the **Quantity to Release** field and set it to **1000**



5.2.4. Define a Bimolecular Reaction

- Click the **Reactions** button.

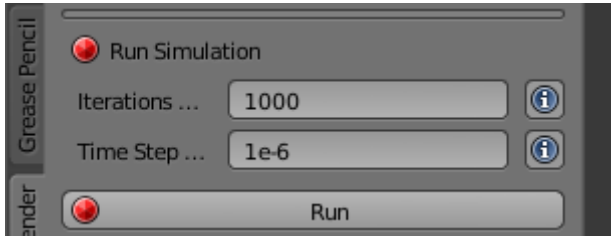
- Change the **Reactants** text field from **a** to **a + b**
- Type **5e3** in the **Forward Rates** text field



5.2.5. Simulate the Model

- Click the **Run Simulation** button

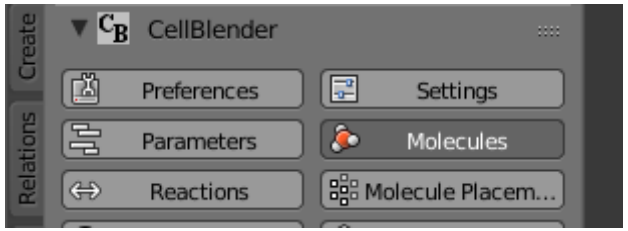
- Change the **Time Step** to **1e-5**
- Click the **Run** button



- Wait for the simulation to complete
- Press the "Reload Visualization Data" button to load the results of the simulation.

5.2.6. Change the Shape of "b"

- Click the **Molecules** button



- Open the **Display Options** subpanel if it isn't already
- Change the **Cone** to **Sphere_2**
- Change the **Scale** to **2.5**
- Change the color to a bright red

5.2.7. View the Results

- Press the "Play" () button below the time line

5.2.8. Save Your File

- **File** > **Save**