Simulating Molecules

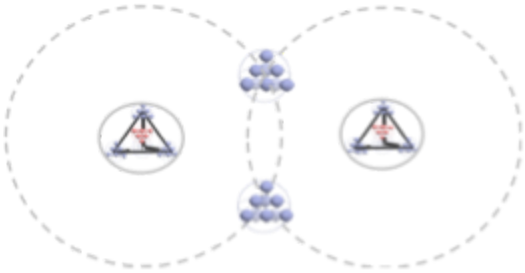
Phase 5 Requirements

Simulating Molecules

Initial Conditions | Runtime | Validation

Objective

To simulate the bonding of atoms sharing electrons and creating molecules. Molecular hydrogen (H_2) should form during this phase. The common molecules for water and air will also be validated in this phase.



Validation Criteria

The following should be validated in this phase of the project:

1. Formation of a simple hydrogen bond (H_2).
2. Formation of a water molecule (H_2O).
3. Formation of air molecule components (N_2 and O_2).

Custom Simulator vs Blender Add-On

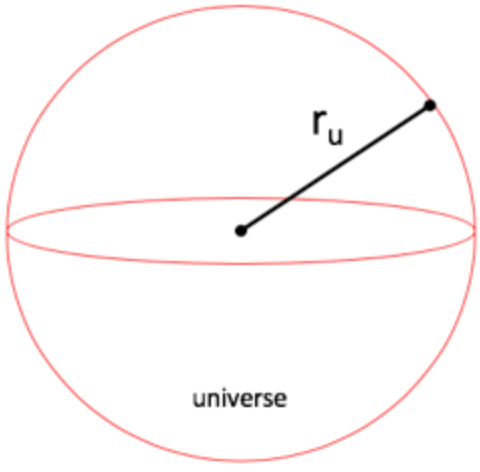
These requirements are intended for developers building a custom simulation. The Quantum Microscope for Blender Add-On was developed using these requirements but were adjusted for scale and Blender's capabilities. The modifications for Blender are found at the end of each section (Initial Conditions, Runtime and Validation). A list of suggested improvements for the Add-On are found in the source code and their ReadMe files.

Initial Conditions

The initial conditions from phase four should be used for this phase with the exception of the following changes and additions.

5.1 Universe Size

For phase five, the size of the simulated universe will need to support molecule formation. The radius (r_u) should be set to at least 10^{-7} meters.



5.2 Number of Hydrogen Atoms

Similar to previous phases, the simulation may be run from scratch by randomly placing wave centers into the simulation, replicating the steps from all other phases. This method will take time to build standalone particles, then composite particles, then atoms and finally molecules.

An alternative method to save time is to randomly inject hydrogen atoms into the simulation, since it has been proven in previous phases, along with all of its components.

If the *Hydrogen Count in Simulation* is 1 or more, then hydrogen atoms are randomly placed into the simulation using hydrogen's properties found in phase four.

Why? *Injecting hydrogen atoms initially into the simulation saves the program time to reach this step.*

5.3 Initial Wave Amplitude

This phase will need a minimum of two nitrogen (N) and three oxygen (O) atomic nuclei. For this to occur, there needs to be sufficient energy and time for these heavier elements to form with 7 protons and 8 protons respectively (not including neutrons).

The suggested method to achieve this is to use the *Spacetime Initial Amplitude* from phase four that was found to allow heavier nuclei to form. But a difference between phase four and five is that the amplitude should not decrease until a minimum of two nitrogen (N) nuclei and three oxygen (O) nuclei are detected in the simulation, if not more. Once detected, energy is decreased using the time property of *Spacetime Initial Amplitude* until reaching the same default *Spacetime Wave Amplitude* property from phase four. The latter wave amplitude may be adjusted if molecules are not forming as expected.

Blender Add-On Modifications

The Quantum Microscope Add-On for Blender uses these requirements with the following modifications:

1. Instead of an option to scale the universe, the various phases are set as different modules in the Blender Add-On with different scaling properties for each phase. At this phase, hydrogen's diameter is set to 200 meters as the baseline for scaling.
2. An External Force is used instead of amplitude, set with different values for nuclear, collision and supernova to simulate what occurs at increasing energy levels for atoms.

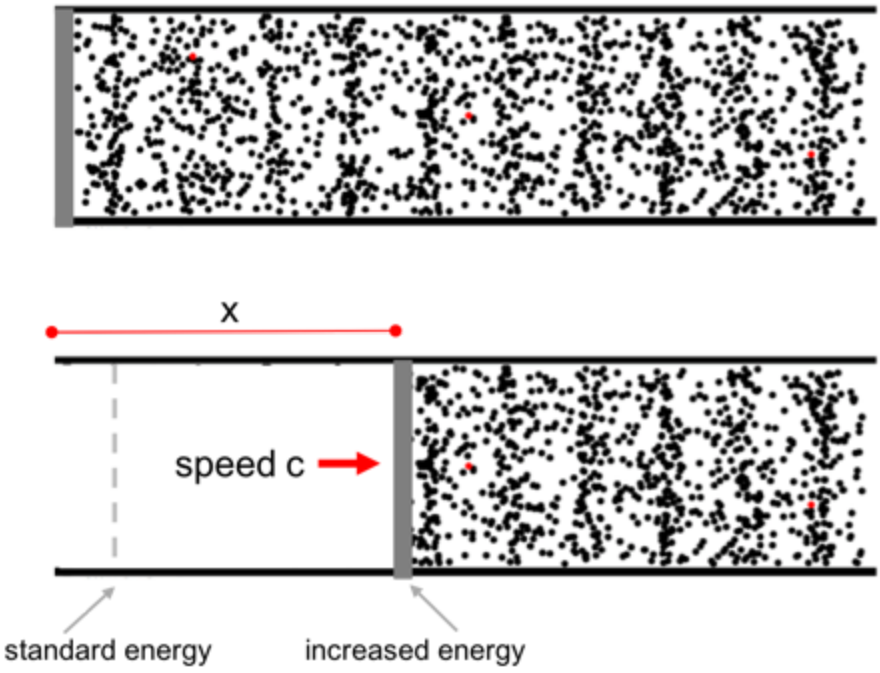
Runtime

The first molecules should bind by sharing electrons during runtime.

5.4 Energy Level

Molecules should bind at energy levels similar to the *Spacetime Wave Amplitude* property set in phase four. However, heavier elements need to form from hydrogen, requiring higher energies at the start of runtime to create nitrogen (N) and oxygen (O).

The runtime will maintain an energy level defined by the *Spacetime Initial Amplitude* property and remain at this value until at least two nitrogen nuclei and three oxygen nuclei are detected in the simulation. After this is achieved, the energy is decreased according to the time defined by the *Time to Amplitude* property until reaching the *Spacetime Wave Amplitude* property.



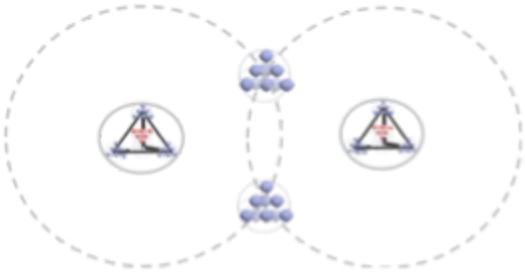
Why? *Nitrogen and oxygen atoms need to form in this phase for validation, before decreasing energy. An alternative, if this is difficult to achieve in runtime, is that these atoms may be randomly placed in the simulation.*

5.5 Physics of Motion

The physics from previous phases should remain unchanged. New interactions are described here as molecules form.

Molecule Formation

The electric force (F_e) and the magnetic orbital force (F_o) equations model the attractive and repulsive forces that form orbitals, validated in phase four. Atoms that are not electrically or magnetically neutral should have motion to reduce wave amplitude, resulting in atoms sharing electrons and binding to become molecules. This should occur naturally at runtime once energy levels are decreased to allow atoms to form. An example is shown below with two hydrogen atoms bonding by sharing two electrons.



Molecular hydrogen (H_2)

Blender Add-On Modifications

The Quantum Microscope Add-On for Blender allows this runtime execution with the following modifications:

1. Molecular hydrogen forms as the attraction of two hydrogen atoms grouped together in Blender particle emitters.
2. Helium is created from hydrogen atoms when the External Force is set to nuclear, but this is animated and does not fuse a helium nucleus due to the issue from Phase 4 with the arrangement of atomic nuclei.

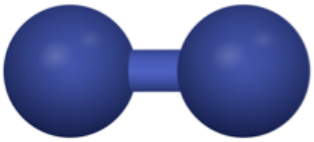
The issues are further documented in the ReadMe file.

Validation

The following should be validated during the simulation.

5.6 Formation of Molecular Hydrogen (H_2)

Molecular hydrogen should form from two hydrogen (H) atoms binding together.



Validation

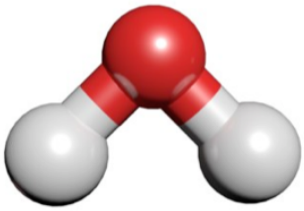
The simulation should confirm the presence of two hydrogen atoms sharing two electrons at runtime and report upon:

- Molecule name
- The geometric arrangement of the atoms in the molecule
- The orbital distance of shared electrons in the molecule

Validate: The above properties of H_2 validated against known sources

5.7 Formation of a Water Molecule (H_2O)

Water should form from two hydrogen (H) atoms binding together along with one oxygen (O) atom.



Validation

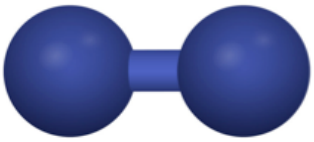
The simulation should confirm the presence of two hydrogen atoms and an oxygen atom bound by shared electrons at runtime and report upon:

- Molecule name
- The geometric arrangement of the atoms in the molecule
- The orbital distance of shared electrons in the molecule

Validate: The above properties of H_2O validated against known sources.

5.8 Formation of Air Molecule Components (N_2 and O_2)

Air consists of different molecules. Two of the common molecules in air are N_2 and O_2. These two molecules will be validated separately.



Validation

The simulation should confirm the presence of two nitrogen atoms sharing electrons at runtime. It should also confirm the presence of two oxygen atoms sharing electrons at runtime and then report upon:

- Molecule name
- The geometric arrangement of the atoms in the molecule
- The orbital distance of shared electrons in the molecule

Validate: The above properties of N_2 and O_2 validated against known sources

5.9 Destruction of Molecules, Atoms and Nuclei (Optional)

Once everything has been validated, the simulation may be run to break apart molecules, atoms and nuclei. This can be achieved by increasing energy (increasing wave amplitude), such as the value found in phase three.

Note: *This section is "extra credit". Once the simulation is built, adding energy to molecules and atoms replicates processes seen on Earth when molecules change when energy (heat) is added; when atomic nuclei are split as more energy is added; or when nucleons split to become quarks as found in particle accelerators.*

Potential experiments to replicate:

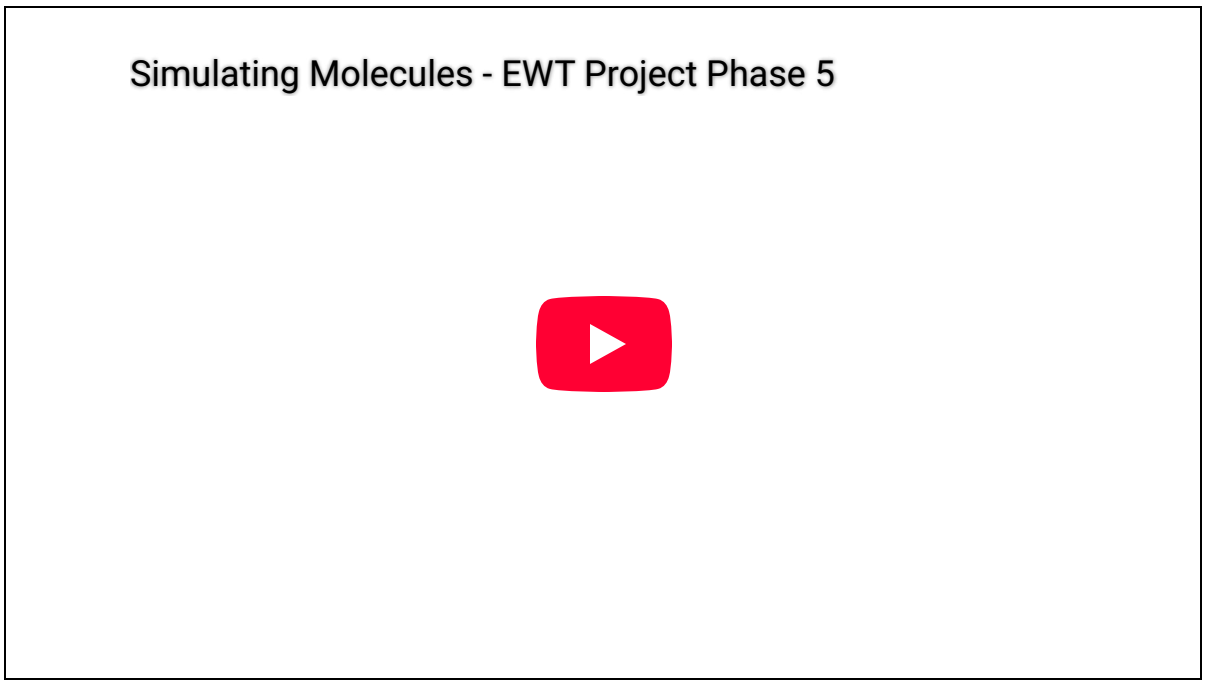
1. Apply energy to molecules and detect molecular binds breaking to separate atoms
2. Apply more energy and detect atomic nuclei separation
3. Apply more energy and detect protons and neutrons separating to become quarks (i.e. electrons and positrons)

Blender Add-On Validation

The Quantum Microscope Add-On for Blender has issues with validating:

1. Water and Air molecules. Due to the issue from Phase 4 generating accurate atomic nuclei, which itself is dependent on the creation of standing waves, only hydrogen atoms are currently simulated. Oxygen and nitrogen atoms may be added after resolving the formation of nuclei.

Video Summary



Previous: Simulating Atoms