Simulating Atoms

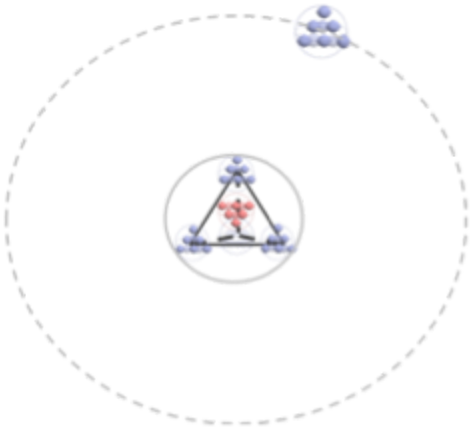
Phase 4 Requirements

Simulating Atoms

Initial Conditions | Runtime | Validation

Objective

To simulate the interaction between protons and electrons, including their orbitals and the formation of the atoms. The hydrogen atom should form during this phase.



Validation Criteria

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

1. Formation of the hydrogen atom.
2. Formation of composite nucleons, creating atoms from helium and larger.
3. Detection of orbitals and expected distances and shapes.

Custom Simulator vs Blender Add-On

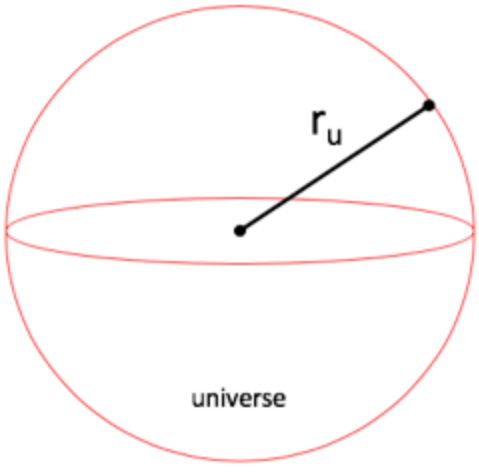
These requirements are intended for developers building a custom simulation. The Quantum Microscope for Blender Add-On was developed using these requirements but were adjusted for scale and Blender's capabilities. The modifications for Blender are found at the end of each section (Initial Conditions, 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 three should be used for this phase with the exception of the following changes and additions.

4.1 Universe Size

For phase four, the size of the simulated universe will need to support atom formation. The radius (r_u) should be set to at least 10^{-9} meters.



Why? *Hydrogen's ground state, the Bohr radius, is 10^{-11} m, the distance between the proton and the electron. Other atoms have electrons that extend further from the nucleus.*

4.2 Number of Protons

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

An alternative method to save time is to randomly inject protons into the simulation, along with electrons and wave centers, since all of these particles should have been proven in previous phases.

If the *Proton Count in Simulation* is 1 or more, then protons are randomly placed into the simulation using the proton properties (geometric configuration) found in phase three.

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

4.3 Initial Wave Amplitude

For the first atom to form (hydrogen), the spacetime amplitude needs to be at an energy level that allows electrons to bind to protons. However, this phase also simulates the production of atoms heavier than hydrogen, which form at energy levels found in stars. The *Spacetime Initial Amplitude* property will be set to be high enough for these atomic nuclei to form and then reduced to be an energy level that allows atoms to form. This property may be iterated upon, as explained in the runtime requirements.

Blender Add-On Modifications

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

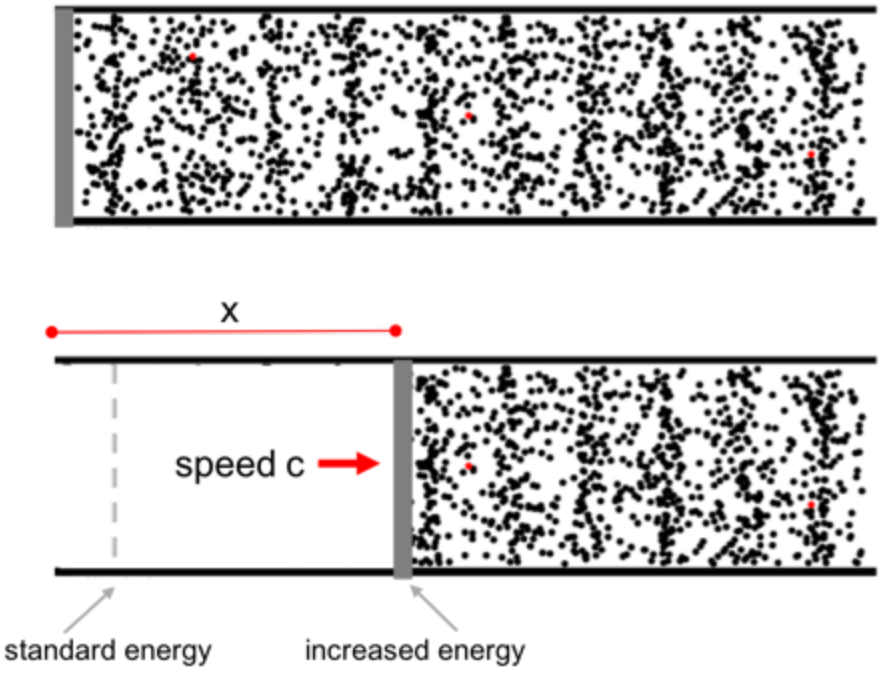
1. Instead of an option to scale the universe, the various phases are set as different modules in the Blender Add-On with different scaling properties for each phase. At this phase, the electron's diameter is set to 0.25 meters as the baseline for scaling.
2. A number of protons, neutrons and electrons are all configurable in the Add-On to allow for different types of atoms, including ionized versions. However, only proton count up to 20 is currently allowed due to the inability to calculate electron orbitals beyond calcium.
3. An option to show the electron's probability cloud has been added, where the nucleus affects a single electron in an orbital, but the electrons do not affect each other (to simulate their position over time).

Runtime

The first atom (hydrogen) should naturally form during runtime. Heavier atoms, beginning with helium, should form over time with sufficient energy.

4.4 Decreased Energy Level

The energy from Step 3.2 can be decreased in phase four, beginning with the same energy level in Step 2.1. The *Spacetime Initial Amplitude* may be increased or decreased from the Step 2.1 value with various iterations until various elements are formed. This step is modeling the energy level in stars that create atomic elements as protons and neutrons bind to become helium and heavier elements.



Why? *Energy levels that create protons (from phase 3) are likely too high for atoms to form, as electrons are more likely to merge with other electrons. When brought down to lower energy levels, the electron should be attracted to a proton but repelled to stay in orbit. This is the first atom – hydrogen.*

4.5 Physics of Motion

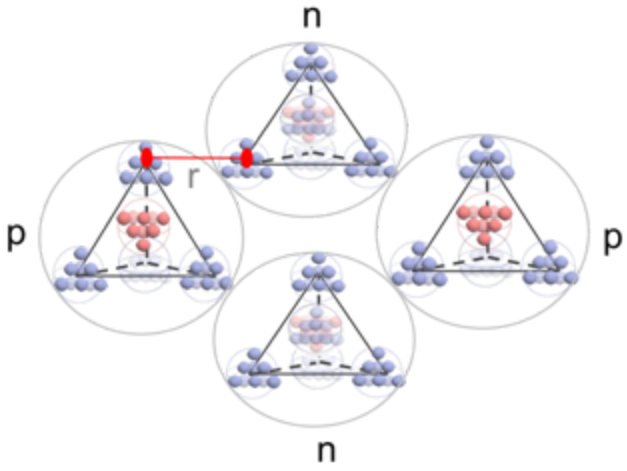
The physics from previous phases should remain unchanged. New interactions are described here as atomic nuclei and atoms form.

Nucleus Formation

The physics of nucleon formation should continue to be the rule of wave centers moving to minimize amplitude, described in phase one. It occurs with wave centers creating standalone particles in phase two, with standalone particles creating composite particles in phase three, and now with composite particles combining to form the nucleus of an atom.

Similar to phase three, there needs to be sufficient energy to push nucleons together, until wave centers within these nucleons reach standing wave nodes. In addition to the initial energy set in the *Spacetime Initial Amplitude* property, the *Time to Amplitude* property needs

to be long enough to allow the probability of nucleons randomly colliding and merging to form heavier elements. For example, a potential arrangement for the second element (helium) is illustrated below with two protons and two neutrons. The runtime *Time to Amplitude* property should allow sufficient time at higher energies to allow two neutrons to merge with a proton, and then a second proton, to form helium. For elements beyond helium, more time will need to be added.



Potential helium arrangement (p – proton; n – neutron)

Certain geometrical alignments will allow nucleon stability and be responsible for the periodic sequence seen in atomic elements. As elements form, their geometries should be recorded.

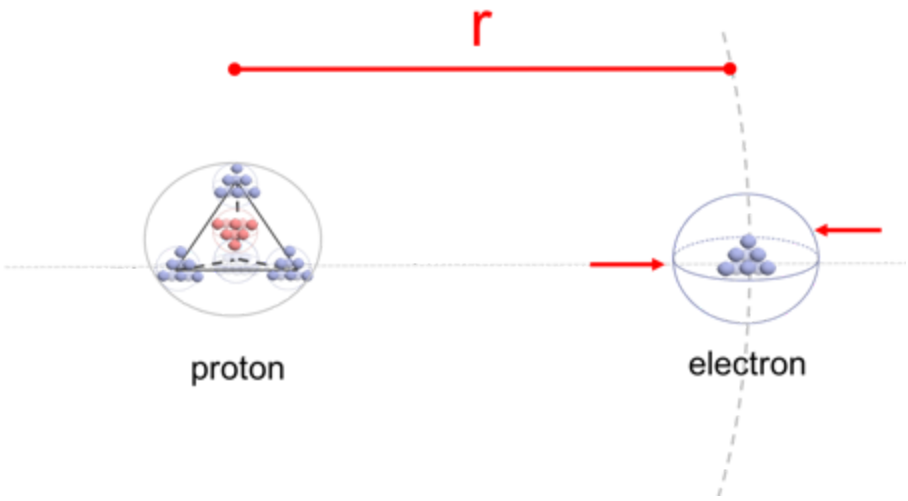
In the previous illustration, a **distance r** is shown between a standalone particle in the proton to the left and one in the neutron on the top. The attractive force that binds the nucleons is the same equation used for the strong force in Step 3.9, except the distance will now be longer to separate nucleons. This is known as the nuclear force. The positrons in both protons repel and the attractive nuclear force *must be greater* than the repelling electric force of the center positron in the protons.

Atom Formation

As energy decreases in the simulated universe, managed by the initial energy (*Spacetime Initial Amplitude* property), the final energy (*Spacetime Amplitude* property) and the time to achieve the final energy (*Time to Amplitude* property), atoms will eventually form when the

energy level decreases to allow electrons to bind with protons without being forced out of orbitals.

Within a proton, the **electric force (F_e)** described in detail in Step 2.9 will attract the electron. When at dipole alignment of the particles within the proton, the **magnetic orbital force (F_o)** described in Step 3.10 will repel the electron. This causes a position for the electron away from the proton that creates an orbital, and it will continuously be pushed and pulled creating orbital shapes.



Atoms and orbitals

When atoms are detected in the simulation, the electron's position should be tracked and charted. The resulting orbitals can be validated against known orbitals.

Blender Add-On Modifications

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

1. The decreasing energy level is not necessary because a separate module was developed for Atoms. It assumes *normal* energy levels.
2. The atom's nucleus forms, but is not the expected arrangement due to the lack of standing wave and node formation.
3. The attractive and repulsive forces from the nucleus is aggregated to a single point at the atom's center, as opposed to each particle, because of the nuclei arrangement issue

from #2.

4. Electrons are affected by the nucleus and by other electrons in their orbitals, but not by electrons in other orbitals.

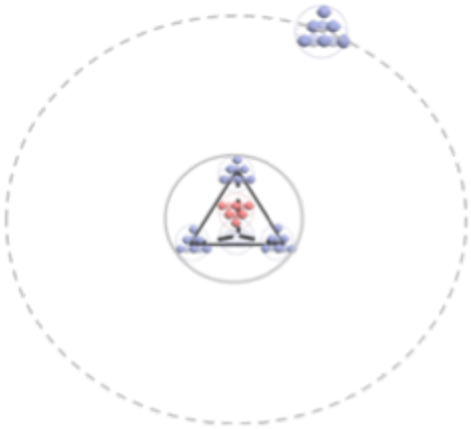
These issues are further documented in the ReadMe file.

Validation

The following should be validated during the simulation.

4.6 Formation of Hydrogen

The bonding of a single proton and a single electron forms hydrogen. It should appear as energy levels decrease such that an electron will remain in an orbital without be expelled from the atom.



Hydrogen atom

Validation

The electron will have a probability cloud, which should be validated and graphed as its position relative to the proton over time. The most probable distance of the electron from the

proton will occur at the alignment of dipoles in the proton, when the electric force and magnetic orbital force cancel. This distance is known as the **Bohr radius (a_0).** This distance should be validated:

Validate: $a_0 \approx 5.3 \times 10^{-11}$ meters

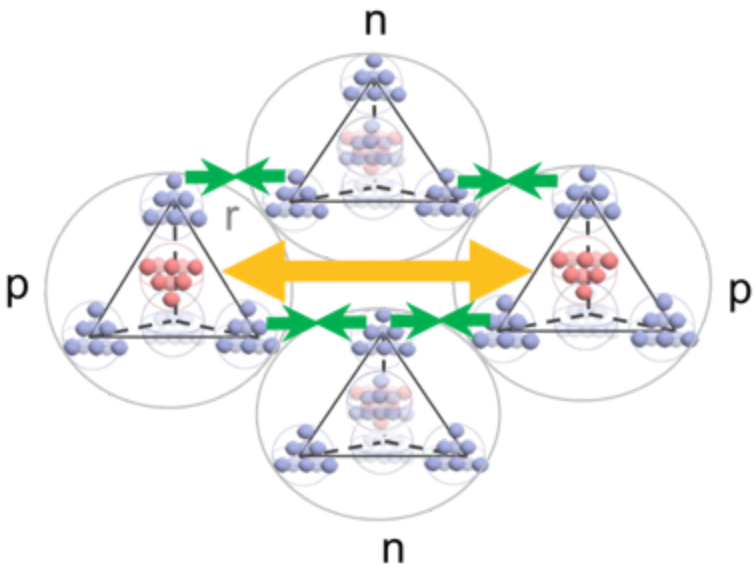
Note: the electron's position in hydrogen is determined by setting the electric force (F_e) and the magnetic orbital force (F_o) to be equal. For a single proton and electron, when solving for distance (r) in the following equations, the result is the Bohr radius.

$$F_e = F_o = \mu_0 c^2 \left(\frac{q_P^2}{4\pi r^2} \right) \alpha_e = \mu_0 c^2 \left(\frac{r_e q_P^2}{\alpha_e 4\pi r^3} \right)$$

4.7 Formation of Heavier Atoms

Heavier atoms, beginning with helium, should form and be validated. The number of heavier atoms will be dependent on the length of time the simulation has sufficient energy for nucleons to combine.

Protons may merge together when separated by neutrons. The following illustrates a potential arrangement for helium (two protons and two neutrons). The **electric force (F_e)** is shown as a repelling yellow arrow. The **nuclear force (F_s)** is shown as attractive green arrows. The nuclear force *must be greater* than the electric force for nucleons to combine. And the geometrical arrangement must place the particles within these nucleons at standing wave nodes to be stable.



Helium nucleus (p – proton; n – neutron)

Validation

The **nuclear force (F_s)** binding nucleons should be the same strong force equation from phase three, but at a larger separation distance. The standalone particles at the vertices of the nucleon particle should be separated at a distance (r) and the force will be:

$$F_s = \mu_0 c^2 \left(\frac{q_P^2}{4\pi r^2} \right)$$

Where:

- μ_0 – the magnetic constant
- q_P – the Planck charge
- α_e – the fine structure constant
- c – the speed of light

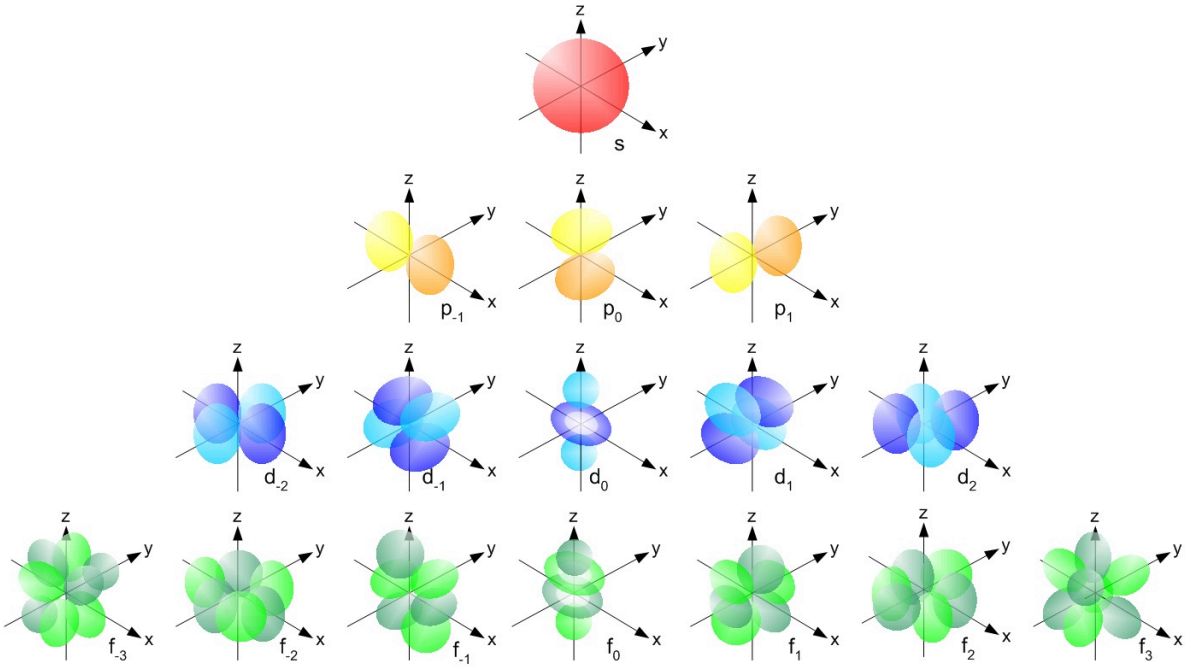
The following should be reported for each atomic element, including ionized elements:

- Atom name
- Geometric arrangement of each nucleon
- The electric force (Fe) value between protons

- The magnetic orbital force (F_o) value between each nucleon

4.8 Formation of Electron Orbitals

Electrons should create unique shapes for each atomic element, based on the electron's configuration in orbital subshells known as s, p, d and f. Due to the alignment of protons in the electron, spherical shapes will change to become *lobes* at certain alignments. More details here. The electron's probability is due to forces that continually attract and repel, similar to hydrogen, becoming more complex for heavier elements as more forces are considered from additional particles.



Validation

The following should be reported for each atomic element, including ionized elements:

- Atom name
- The most probable location of each electron within the atom
- The orbital shape (graphed position over time) of each electron within the atom

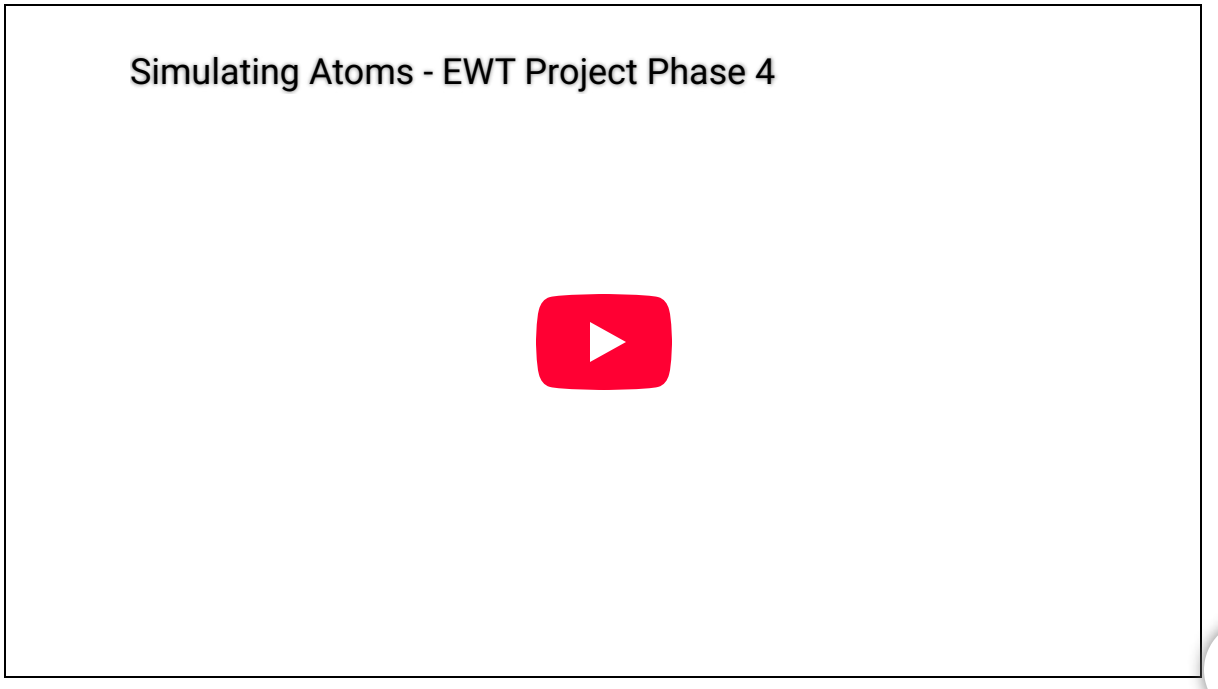
Validate: The outermost electron's location of each element to the atomic radius found at www.webelements.com within an accuracy of +/- 20%. *Electron distances are difficult to measure and this level of accuracy will be acceptable for validation.*

Blender Add-On Validation

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

1. Orbital distances and energies from simulation properties. The distances and energies of orbitals is pre-calculated using a separate solver for simultaneous equations. This solver needs to be moved into Blender python scripts to calculate in real-time in the simulation vs pre-calculated.
2. Nuclear force. Similar to the issue calculating the strong force in the previous phase, standing longitudinal waves and transverse waves need to be accurately modeled first in Phase 1 for this to be calculated.

Video Summary



Previous: Simulating Composite Particles **Next: Simulating Molecules**