Subatomic Sandbox Simulator

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November 1, 2023

1 Establishing a system of units

As we are working on atomic scales, we shall find it useful to select non-standard units. This involves both choosing different quantities to form the base units of our system and subdividing the units to better suit the size of our measurements. The set of units we shall find most advantageous to use are as follows.

Measurement	Unit	S.I. Conversion
Time	Picoseconds (ps)	$1\text{s} = 10^{12}\text{ps}$
Length	Picometres (pm)	$1\text{m} = 10^{12}\text{pm}$
Mass	MeV per c squared (Mev/c^2)	$1\text{kg} = 5.6164 \times 10^{29}\text{Mev/c}^2$
Charge	Microelementary charge (μe)	$1\text{C} = 6.2414 \times 10^{24}\mu\text{e}$
Temperature	Kelvin (K)	1K = 1K

1.1 Changing the base

The seven S.I. base units are seconds, metres, kilograms, amperes, kelvin, candela, and moles, though we shall disregard the last two of these as we are unlikely to find a reason to interact with luminous intensity or amounts of substance in particle simulations. We may write any unit that we are likely to encounter in the form

$$\text{s}^{n_1}\text{m}^{n_2}\text{kg}^{n_3}\text{A}^{n_4}\text{K}^{n_5}$$

and if we set out that this is the standard order of the S.I. units, we may abstract any unit into the form of a $\mathbb{R}^5$ vector whose components are the exponents n_i. In this application, vector addition becomes multiplication of units while scalar multiplication becomes raising units to different powers. One may verify that all of the required properties of vector arithmetic (commutativity, associativity, etc.) hold when vectors are applied in this way and so we may immediately apply a range of ideas from linear algebra.

One particular idea that we wish to use is that of changing basis. If we take the basis vectors $\vec{e}_1, \cdots, \vec{e}_5$ to be the S.I. base units, changing to a different set of base units is simply a change of basis vectors, practically the definition of matrix-vector multiplication. As such, if we create a matrix which encodes our change of base units, we may use this to easily convert any units we come across from S.I. to our new system.

The only unit which we fundamentally change (i.e. the quantity that the unit measures is different) is that of current. We change this unit for that of charge and so we must use the formula $I = Qt^{-1}$ to convert units (within some constant factor which shall be dealt with later). We therefore wish for the vector $\vec{e}_4$ (initially current) to go to itself (now symbolising charge) minus the time vector $(-\vec{e}_1)$; in other words,

$$U\vec{e}_4 = \vec{e}_4 - \vec{e}_1 = \begin{bmatrix}0\\0\\0\\1\\0\end{bmatrix} - \begin{bmatrix}1\\0\\0\\0\\0\end{bmatrix} = \begin{bmatrix}-1\\0\\0\\1\\0\end{bmatrix}.$$

As all other units are maintained (i.e. $U\vec{e}_i = \vec{e}_i$ when $i \neq 4$) we may therefore summarise

the change of basis in the form of the matrix

$$U = \begin{bmatrix} 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}. \tag{1}$$

This matrix allows us to convert units given in the standard S.I. quantities into our system of measured quantities. However, we shall need to exercise care during this process due to the appearance of certain constant factors. If we initially convert current in amperes to charge in coulombs, we can avoid this issue as there is a one-to-one correspondence between ampere-seconds and coulombs. We are then free to substitute in equivalences between different units of the same measurement (e.g. seconds and picoseconds, coulombs and elementary charge, etc.) to subdivide our units as we desire.

1.2 An example (Converting the permittivity of free space)

The permittivity of a vacuum, ϵ_0, is approximately equal to $8.8541 \times 10^{-12}\ \mathrm{F \cdot m^{-1}}$. In terms of the S.I. units, $1\mathrm{F} = 1\mathrm{s}^4\mathrm{m}^{-2}\mathrm{kg}^{-1}\mathrm{A}^2\mathrm{K}^0$, we may therefore represent the unit of farads per metre via the following vector.

$$\vec{F} - \vec{m} = \begin{bmatrix} 4 \\ -2 \\ -1 \\ 2 \\ 0 \end{bmatrix} - \vec{e}_2 = \begin{bmatrix} 4 \\ -3 \\ -1 \\ 2 \\ 0 \end{bmatrix}$$

Application of our unit transformation matrix yields the representation

$$U \begin{bmatrix} 4 \\ -3 \\ -1 \\ 2 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 4 \\ -3 \\ -1 \\ 2 \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \\ -3 \\ -1 \\ 2 \\ 0 \end{bmatrix}$$

in our new system. That is to say, we may represent farads per metre in the form[1] $\mathrm{s}^2\mathrm{m}^{-3}\mathrm{kg}^{-1}\mathrm{C}^2\mathrm{K}^0$.

We may now begin subdividing our units. There is no elegant way like that found for quantity conversion to do this; as such, we must resort to substitution of unit equivalences.

$$\begin{aligned} \mathrm{F \cdot m} &= \mathrm{s}^2\mathrm{m}^{-3}\mathrm{kg}^{-1}\mathrm{C}^2\mathrm{K}^0 \\ &= \left(10^{12}\mathrm{ps}\right)^2 \left(10^{12}\mathrm{pm}\right)^{-3} \left(5.6164 \times 10^{29}\mathrm{Mev/c^2}\right)^{-1} \left(6.2414 \times 10^{24}\mu\mathrm{e}\right)^2 \mathrm{K}^0 \\ &= \frac{6.2414^2}{5.6164} \times 10^{(24-36-29+48)}\ \mathrm{ps}^2\mathrm{pm}^{-3} \left(\mathrm{MeV/c^2}\right)^{-1} \mu\mathrm{e}^2\mathrm{K}^0 \\ &= 6.9360 \times 10^7\ \mathrm{ps}^2\mathrm{pm}^{-3} \left(\mathrm{MeV/c^2}\right)^{-1} \mu\mathrm{e}^2\mathrm{K}^0 \end{aligned}$$

[1] As we have worked with time in seconds, current in amperes, and charge in coulombs, we have no constant conversion factor introduced by this transformation.

Now that we have fully converted the given units into our preferred system, we may convert the constant.

$$\begin{aligned}\epsilon_0 &\approx 8.8541 \times 10^{-12}\ \mathrm{F \cdot m^{-1}} \\ &= 8.8541 \times 10^{-12} \times \left(6.9360 \times 10^{7}\ \mathrm{ps^2 pm^{-3}} \left(\mathrm{MeV/c^2}\right)^{-1} \mu\mathrm{e^2 K^0}\right) \\ &= 6.1412 \times 10^{-4}\ \mathrm{ps^2 pm^{-3}} \left(\mathrm{MeV/c^2}\right)^{-1} \mu\mathrm{e^2} \end{aligned} \tag{2}$$

2 Approximate mechanics

We shall often find situations when considering interactions between multiple bodies where finding analytic solutions to our equations is impractical or completely impossible. As such, we need to develop an approximate approach to solving the equations of our simulation numerically.

Assume we have some non-constant (i.e. time-varying) acceleration $\vec{a}(t)$ acting upon a particle. If function varies reasonably slowly such that within some small time Δt it is almost constant, we may segment our simulation into myriad "frames" of some small duration over which acceleration is taken to be constant.[2]

Take $\vec{a}(t)$ to be equal to some constant $\vec{\alpha}_t$ over the interval t to $t + \Delta t$. We may find the velocity at the end of this interval by incrementing the initial velocity by the integral of the constant acceleration over the interval.

$$\vec{x}'(t + \Delta t) = \vec{x}'(t) + \int_t^{t+\Delta t} \vec{\alpha}_t \, d\tau = \vec{x}'(t) + \vec{\alpha}_t \Delta t$$

Similarly, the position at the end of the interval may be found by integrating again.

$$\vec{x}(t + \Delta t) = \vec{x}(t) + \int_t^{t+\Delta t} [\vec{x}'(t) + \vec{\alpha}_t \Delta t] = \vec{x}(t) + \vec{x}'(t)\Delta t + \frac{\Delta t^2}{2}\vec{\alpha}_t$$

We therefore have the following system of equations for approximating our system in small time steps.

$$\begin{cases} \vec{x}'(t + \Delta t) = \vec{x}'(t) + \vec{x}''(t)\Delta t \\ \vec{x}(t + \Delta t) = \vec{x}(t) + \vec{x}'(t)\Delta t + \dfrac{\Delta t^2}{2}\vec{x}''(t) \end{cases}$$

3 Electrostatic interactions

For the purposes of this section, suppose we have n point charges with positions $\vec{x}_i$, masses m_i, and charges q_i. We shall be using classical electromagnetism (i.e. Coulomb's Law, Faraday's Law, Gauss's Law, etc.).

3.1 Visualising the electric field

To visualise the electric field, we sample a set of points and calculate the contribution of each particle at said point. The electric field induced by a single particle is given by the equation

$$\vec{E} = \frac{q}{4\pi\epsilon R^2}\hat{R} \tag{3}$$

[2] It shall be seen that this line of reasoning leads to two of the usual SUVAT equations.

where $\hat{R}$ is the unit vector in the direction away from the particle, R is the distance from the particle, and ϵ is the permittivity of the material (if instead electric flux density is used, this factor may be removed).

We may break down the overall electric field and view it as the sum of the interactions of each particle $\vec{x}_i$ on each sample point $\vec{r}$; we shall call this $\vec{E}_i$. The vector from $\vec{x}_i$ to $\vec{r}$, $\vec{R}_i$, is $\vec{r} - \vec{x}_i$. From this,

$$||\vec{R}_i|| = ||\vec{r} - \vec{x}_i||, \tag{4}$$

$$\hat{R}_i = \frac{\vec{R}_i}{||\vec{R}_i||} = \frac{\vec{R}_i}{||\vec{r} - \vec{x}_i||}. \tag{5}$$

Substituting these expressions into the general electric field formula, we arrive at the formula

$$\vec{E}_i = \frac{q_i \hat{R}_i}{4\pi\epsilon||\vec{R}_i||^2} = \frac{q_i}{4\pi\epsilon||\vec{r} - \vec{x}_i||^2} \frac{\vec{r} - \vec{x}_i}{||\vec{r} - \vec{x}_i||}. \tag{6}$$

To find the overall electric field at each sample point $\vec{r}$, we sum the contributions of each particle.

$$\begin{aligned} \vec{E}(\vec{r}) &= \sum_i \vec{E}_i \\ &= \sum_i \left[\frac{q_i}{4\pi\epsilon||\vec{r} - \vec{x}_i||^2} \frac{\vec{r} - \vec{x}_i}{||\vec{r} - \vec{x}_i||} \right] \\ &= \frac{1}{4\pi\epsilon} \sum_i q_i \frac{\vec{r} - \vec{x}_i}{||\vec{r} - \vec{x}_i||^3} \qquad \left(= \frac{1}{4\pi\epsilon} \sum_i \frac{q_i}{(\vec{r} - \vec{x}_i)^2} \frac{\vec{r} - \vec{x}_i}{||\vec{r} - \vec{x}_i||} \right) \end{aligned} \tag{7}$$

3.2 Acceleration due to charged interactions

The formula for finding the magnitude and direction of the electric field which we found in the previous section, (7), shall prove useful in finding the force acting on each charged particle due to every other one. The electric field acts to display the force acting upon a virtual particle of charge $+1C$ at each position. We may therefore find the force applied to each of our real particles via the relation $\vec{F}(\vec{x}_i) = q_i \vec{E}(\vec{x}_i)$.

Until now, we have been considering snapshots of time in which particles do not move. In reality, we will have to evaluate our forces and, by extension, the electric field at several different times. This means that our equations for the electric field and the electric force should actually be

$$\vec{E}(\vec{x}_i, t) = \frac{1}{4\pi\epsilon} \sum_{j \neq i} \frac{q_j}{[\vec{x}_i - \vec{x}_j(t)]^2} \frac{\vec{x}_i - \vec{x}_j(t)}{||\vec{x}_i - \vec{x}_j(t)||}, \quad \vec{F}(\vec{x}_i, t) = q_i \vec{E}(\vec{x}_i, t).$$

Using Newton's Second Law of Motion in vector form, $\vec{F} = m\vec{a} = m\vec{x}''$, we arrive at the differential equation

$$\frac{d^2\vec{x}_i}{dt^2} = \frac{\vec{F}(\vec{x}_i, t)}{m_i} = \frac{q_i}{m_i} \vec{E}(\vec{x}_i, t).$$

This equation is likely to be impossible to solve analytically. As such, methods of numerical approximation must be employed.

If we apply the methods of Section 2, we arrive at the two stepwise formulae

$$\vec{v}_i(t+\Delta t) = \vec{v}_i(t) + \frac{\vec{F}(\vec{x}_i(t),t)}{m_i}\Delta t \tag{8}$$

$$\vec{x}_i(t+\Delta t) = \vec{x}_i(t) + \vec{v}_i(t)\Delta t + \frac{\vec{F}(\vec{x}_i(t),t)}{2m_i}\Delta t^2 \tag{9}$$

By applying these formulae recursively and starting at $t = 0$, we find the formulae

$$\vec{v}_i(n\Delta t) = \vec{v}_i(0) + \Delta t \sum_{k=0}^{n-1} \vec{F}\left(\vec{x}_i(k\Delta t), k\Delta t\right),$$

$$\vec{x}_i(n\Delta t) = \vec{x}_i(0) + \Delta t \sum_{k=0}^{n-1} \vec{v}_i(k\Delta t) + \frac{\Delta t^2}{2m_i} \sum_{k=0}^{n-1} \vec{F}\left(\vec{x}_i(k\Delta t), k\Delta t\right).$$

4 Constructing Protium

We now wish to find a way to model the most basic atom, Protium (a.k.a. Hydrogen-1). This atom consists of two particles - one proton and one neutron - which interact with each other via electrostatic attraction. In order for our atom to be stable, we must initialise the simulation with the orbiting electron moving with some particular orbital velocity perpendicular to the vector from the electron to the atom. To find this velocity, we equate the magnitude of the inwards acceleration that of the centripetal acceleration given by the formula $a_c = v_{\text{orbit}}^2/R$ where R is the orbital radius.

Section 3.2 dictates that the acceleration experienced by our electron due to the charge of the proton is equal to

$$\vec{a}_E = \frac{q_e}{m_e}\vec{E}(\vec{x}_e,t) = \frac{1}{4\pi m_e \epsilon}\frac{q_e q_p}{(\vec{x}_e - \vec{x}_p)^2}\frac{\vec{x}_e - \vec{x}_p}{||\vec{x}_e - \vec{x}_p||} = \frac{q_e q_p}{4\pi m_e \epsilon R^2}\frac{\vec{x}_e - \vec{x}_p}{R},$$

$$||\vec{a}_E|| = \frac{1}{4\pi m_e \epsilon}\frac{|q_e q_p|}{R^2}\frac{||\vec{x}_e - \vec{x}_p||}{R} = \frac{|q_e q_p|}{4\pi m_e \epsilon R^2}.$$

Asserting that this equals the centripetal acceleration allows us to solve for orbital speed.

$$a_c = ||\vec{a}_E||$$

$$\frac{v_{\text{orbit}}^2}{R} = \frac{|q_e q_p|}{4\pi m_e \epsilon R^2}$$

$$v_{\text{orbit}} = \frac{1}{2\sqrt{R}}\sqrt{\frac{|q_e q_p|}{\pi m_e \epsilon}}$$

The values of these constants can be calculated in our units. If we choose to work in free space, ϵ becomes ϵ_0 whose value we already know (see equation (2)). The charges of the proton and electron (q_p and q_e) are $\pm$e respectively which may be converted to $\pm 10^6 \mu$e. Finally, the mass of the electron is equal to 0.511MeV/c^2. This allows us to evaluate all of the constants in this formula, giving

$$v_{\text{orbit}} = \frac{1}{2\sqrt{R}} \times 3.1848 \times 10^6 \text{pm}^{3/2} \cdot \text{ps}^{-1} = \frac{1.5924 \times 10^6}{\sqrt{R}} \text{pm}^{3/2} \cdot \text{ps}^{-1}.$$

At 100pm, $v_{\text{orbit}} = 1.5924 \times 10^6 \text{pm} \cdot \text{ps}^{-1}$.