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Development of a simple algorithm for linear accelerator construction and simulation

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DOI https://doi.org/10.48188/so.4.13 Aim: To develop a simple algorithm that accurately constructs and simulates an Alvarez-type linear accelerator given the initial conditions and number of accelerator parts.

Methods: We wrote the algorithm in Python, a programming language with numerous useful math and science libraries, and the ability to use classes and objects. The particles were accelerated in electric fields (which we assumed to be constant within each cavity at any given moment) to allow for a comparison of numerical results with an analytic expression. No magnetic fields were present in the simulations used in this article, and the particle beams were instead focused by using collimators. The algorithm first constructed the accelerator by guessing the appropriate length of each segment until it found optimal lengths for accelerating most particles in the beam. Once constructed, the accelerator could accelerate beams of particles and the results could be analyzed.

Results: The algorithm successfully constructed multiple different accelerators from the initially given conditions. The first two simulations had arbitrary accelerators in which hydrogen and lead ions were accelerated, and the results were in line with expectations from the analytic solution. The largest simulation was that of CERN's Linac4 accelerator, which produced results similar to those found in the real world.

Conclusion: Significant results could be obtained even with an algorithm as simple as the one described here. The algorithm could be further improved by using a more realistic potential inside the accelerator cavities, and more particles could pass through if magnetic fields which focus the beam were turned on.

Keywords: accelerator; simulation; construction; linac; Alvarez; particles



Introduction

Until the invention of particle accelerators, elementary particles could only be studied by observing cosmic rays. After the invention of the electrostatic particle accelerator, Gustav Ising proposed the first particle accelerator using an alternating voltage source in 1924 [1], which was constructed two years later by Rolf Widerøe [2]. The aim was to let charged particles pass through regions where they would be accelerated by an oscillating electric field during time intervals when the field is directed so as to speed up the particles, after which they would enter drift tubes where they are protected from external fields which would slow them down. When the fields were correctly directed again, the particles would be released into cavities where they are accelerated. The next significant improvement in linear accelerator (linac) technology came after World War 2 with the invention of radio-frequency cavities, which could be used as a voltage source [3]. The first such accelerator was constructed by Alvarez in 1946 [4].

We hypothesized that a simple algorithm that successfully constructs and simulates an Alvarez-type linear particle accelerator could be developed, considering the type of particles used, initial conditions, and the maximum voltage inside the cavities between drift tubes. By utilizing these variables, the algorithm would determine the appropriate length of accelerator parts and the distances between them, focusing on the distances between the tubes where the particle speeds are not constant, which are otherwise harder to find, as the problem cannot be solved analytically. Upon successful construction, the accelerator can be applied to a significantly larger number of particles, allowing for a more detailed analysis of the results, such as examining the energy and velocity distributions of the accelerated beam of particles and assessing the number of particles that successfully passed through the accelerator.

Methods

Relativistic mechanics

Since particles in accelerators can reach very high energies, it is necessary to use relativistic equations of motion. The entire simulation is observed from the laboratory reference frame, and since only charged particles are used, the strongest external force exerted on each accelerated particle in the beam is the external Lorentz force:

$$\vec{F} = q\vec{E} + q\vec{\nu} \times \vec{B} \tag{1}$$

where \vec{F} is the 3-force from classical mechanics, q is the charge of the particle, \vec{v} is the particle velocity, and \vec{E} and \vec{B} are the electric and magnetic fields at a given point in space, respectively. However, we only focused on cases where the magnetic field is set to 0.

All perturbations on the system are ignored, so only the Lorentz force is considered. The 3-acceleration in special relativity is given by [5]:



$$\vec{a} = \frac{1}{m\gamma} \left(\vec{F} - \frac{(\vec{F} \times \vec{v})\vec{v}}{c^2} \right)$$
(2)

where *m* is the mass of the particle, c = 299 792 458 $\frac{m}{s}$, and $\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}$ is the Lorentz factor.

The kinetic energy in high-energy physics can be written as [6]:

$$T = (y - 1) mc^2$$
 (3)

Alvarez linac

The Alvarez linac was the first to make use of radiofrequency (RF) cavities as a voltage source [4], which were needed to achieve frequencies of a few hundred GHz [7]. These types of accelerators, where particles travel down a tube in which they are protected from external electric fields, are called Drift Tube Linac (DTL) [3].

In an Alvarez-type linac, the electric fields between all drift tubes are simultaneously identically directed. This means that, for particles to efficiently accelerate, they need to spend half the period of the voltage source inside the cavities where they are accelerated (which also corresponds to the time interval when the electric field does not change direction) and the other half inside drift tubes, where they are protected from external electric fields which would slow them down (because the electric field is in the opposite direction). Since the particle accelerates, the tubes need to become longer (as do the distances between them), and the length of the *n*-th tube l_n can be written as:

$$l_n = \frac{v}{2f} \tag{4}$$

where v is the particle speed throughout the tube and f is the frequency of oscillation of the electric fields.

The distances between the tubes, where the particle speeds are not constant, are harder to find, which was the purpose of the algorithm described in this study.

Alvarez linac electric field approximation

It is necessary to find the magnitude and direction of the electric field at each point in space before the simulation can start. We used a linear approximation of the potential between drift tubes, which translates to a constant electric field. As for the direction, it is assumed that the electric fields are always parallel to the z-axis. If the potential is defined as 0 at the midpoint between subsequent drift tubes, the potential *V* can be written as:

$$V(z,t) = 2 \frac{z - z_0 - \frac{d}{2}}{d} V_{\max} \cos(\omega(t - t_0))$$
(5)

where $z - z_0$ is the distance from the end of the previous drift tube, and d is the distance between subsequent drift tubes. V_{max} is the maximum magnitude of the potential at a given gap between drift tubes, and the $\cos(\omega(t - t_0))$ term comes from the fact that an oscillatory RF cavity source is used, with an angular frequency $\omega = 2\pi f$. The variable t describes the time



evolution of the potential V(z,t) and it is the time since the beginning of the simulation. t_0 is determined by the algorithm in a way to successfully accelerate a large number of particles, its value is set up in a way such that the electric field changes sign when the beam of particles arrives so that the field can increase the speed of the particles instead of slowing them down.

The electric field in the gaps is taken as the negative gradient of the potential, which gives:

$$E(t) = \frac{2}{d} V_{\text{max}} \sin(\omega(t - t_0))$$
(6)

Algorithm – particle creation

The particles are created at the origin point of the coordinate system (0,0,0) at t = 0. The system is placed so that the particles accelerate in the positive z direction, which is also the symmetry axis of the accelerator. The created particles do not interact with each other, and they have a velocity distribution. Their speeds are generated as normally distributed random variables with a mean and standard deviation set by the person using the algorithm. The velocity direction angles, the polar and azimuthal angles about the z-axis, are generated as evenly distributed random variables.

Algorithm – arbitrary accelerator construction

Before the motion of particles can start, an accelerator has to be constructed. Tubes of arbitrary, user-defined lengths and radii can be added as parts of the accelerator, and the distances between subsequent tubes can also be defined. The program uses these parameters to calculate the z-coordinates of the beginning and end of each accelerator segment and stores them in two separate lists, which are later used to determine whether the particles are inside an electric field. An arbitrarily constructed accelerator is shown in **Figure 1**.



Figure 1. An example of an arbitrarily constructed accelerator with 2 collimators at the ends, and 3 drift tubes in between.



Algorithm – particle motion

The Runge-Kutta 4 (RK4) method [8] is used for numerically solving the equations of motion of the particles. Before moving the particle, it is necessary to check whether it is inside the region where the electric field is non-zero. For this purpose, we introduced two counters: one for counting the number of times a particle entered a new segment and another for counting the number of times the particle left the previous segment. This was done by using the z-coordinate of each particle in every step and checking if the particle crossed the z-coordinate of the start (end) of the next (current) segment. If the particle has entered more segments than it has left, that means that it is inside the drift tube, so the electric field is set to 0. In the other case (the particle has left every segment it has entered), the electric field is given by eq. 6. The times, positions and velocities of each particle in each step are saved for further use in the algorithm. The time step used in each step of moving the particles using the RK4 method was varied throughout the simulations. This is especially useful in cases where the particles start out at non-relativistic speeds and their speeds increase by orders of magnitude during the simulation. Using a constant timestep would either lead to an unnecessary amount of precision at the beginning of the simulation or unreasonable run times. An example of particles going through a collimator, a device used to filter out particles and make the particle beam narrower, is shown in Figure 2. The particles that hit the edge of a collimator (or any other drift tube) are removed from the beam array in the algorithm. The algorithm solves the equations of motion only for the particles which are in the beam array, so the particles in question are removed for the remainder of the simulation.



Figure 2. An example of particles with randomly generated velocities (both in magnitude and in direction) going through a collimator.



Algorithm - finding the optimal accelerator

The first step in finding the optimal accelerator is searching for the particle that should be accelerated the most. It is not enough to take the mean speed of the generated particles, as there are velocity components in the x and y directions as well. We solved this by first allowing the particles to go through the initial collimator and then taking the median *z*-component of the velocity as the initial velocity of the particle that needs to be accelerated the most.

After achieving the desired median velocity, all particles are removed, and a test particle with the median velocity as its initial velocity is created. The test particle first goes through the collimator, after which the electric field is set so that it starts accelerating the test particle when it exits the first collimator. We achieved this by setting t_0 in eq. 6 as the time when the test particle exits the collimator. After this, another segment is added at a distance d from the collimator. The distance d is an informed estimate at first; the particle must stay in the gap between the first collimator and the subsequent drift tube for half of the RF source's period, and the average speed of the particle is somewhere in between the initial speed at the beginning of the cavity and the speed of light. After making the first estimate (a weighted average of the test particle's initial speed and the speed of light), the motion is continued, and the algorithm checks whether the initial guess was good or if it needs to be modified depending on whether the particle crossed the gap before or after the electric field direction change occurred. The condition that the cavity is too long is satisfied when the particle goes through the entire cavity and enters the next drift tube before the electric field changes its sign and starts accelerating the particle. The other case, when the cavity is too short, is satisfied when the electric field changes sign before the particle enters the next drift tube. These conditions are sensical, but would lead to infinite loops when running the program without additional modifications, as no numerical method is entirely accurate. It is thus necessary to define an acceptable distance to the next drift tube by multiplying the initial guess by a positive factor smaller than 1 if the cavity was too long, and in the case where the cavity was too short, its length is multiplied by a factor larger than 1. This kind of algorithm can be seen in the pseudocode below:

```
# d – gap length
```

```
# Emax - maximum electric field magnitude
# E - current electric field magnitude
# Eprev - electric field magnitude in the previous step
# q - particle charge
# z - distance from the end of the previous drift tube
if (|E/Emax| <0.01 and |z/d| <0 .01):
{
  print("The gap is of appropriate length!")
}
else if (E*q<0 and Eprev*q>O):
{
  print("The gap is too short!")
  d *=1.1
```





```
}
else if z>d:
{
print("The gap is too long!")
d*=0.9
}
```

After the gap length is modified, the particle is returned to the end of the previous segment and the checking process repeats. This is done after each drift tube. The length of the drift tube can be easily obtained from eq. 4, as the particle velocity remains constant inside the drift tube.

It is possible to analytically check whether the cavity length is accurate using equation 2. In the cavity, the velocity and the force on the particle are both in the *z*-direction. By taking out the force from the parenthesis, the remaining terms inside it are equal to γ^2 . If the acceleration is written as dv/dt and the force from eqs. 1 and 6 is used, the following differential equation is obtained:

$$\frac{d\nu}{dt} = \frac{q}{m} E(t) \gamma(\nu)^{-3}$$
(7)

which can be solved by separation of variables. The equation is first turned into:

$$\left(1 - \frac{\nu^2}{c^2}\right) d\nu = \frac{2|q|}{md} V_{\max} \sin(\omega(t - t_0)) dt$$
(8)

where the analytic solution is obtained by integrating both sides of the equation. The limits of the integral can be set as v_i and v_f for the left-hand side, and t_i and t_f for the right-hand side. The cosines which come from the integration are easy to discard, as the particle arrives at the beginning of the first cavity at $t = t_0$, and at the beginning of the *n*-th cavity after the first one at $t = t_0 + nT$, so $\cos(\omega(t - t_0))$ every time. The particle comes to the end of each cavity after half a period after it arrives at the beginning, meaning that $\cos(\omega(t - t_0)) = -1$ in this case. Inserting this into the integral of eq. 8, the following result is obtained:

$$\left(1 - \frac{\nu^2}{c^2}\right) d\nu = \frac{2|q|}{md} V_{\text{max}} \sin(\omega(t - t_0)) dt$$
(9)

The numerical result can now be checked with the analytic solution by checking whether the following is true:

$$\frac{\nu_{i} \gamma(\nu_{i}) + \frac{4|q|V_{\max}}{\omega m d}}{\nu_{f} \gamma(\nu_{f})} \approx 1$$
(10)



Results

Simulation with protons

We completed the first simulation with protons. The accelerator, which wer constructed with the algorithm, has two identical collimators at the beginning and the end of the accelerator with a length of 50 cm and radius of 1 cm, and further nine drift tubes in the middle. The electric fields oscillates with a frequency of 300 Mhz, and $V_{\rm max}$ is 50 MV. The particles generated have a mean velocity of 0.08 c with a standard deviation 100 times smaller than the mean. The maximum polar angle of the initial velocity (angle to the z-axis) is 10°.

By allowing the test particle through, the change in its speed agrees with the analytic solution from eq. 10. The test particle accelerated from 0.0802 c to 0.801 c. The distance between the centers of the first two cavities is 206 cm, and the distance between the last two is 494 cm, which also intuitively logical, as the particle gets faster over time.

After successfully constructing the accelerator, a beam of 10,000 protons goes through the accelerator. Overall, 952 emerged from the first collimator with an (arithmetic) average speed of 0.0800 c and a standard deviation of 0.0008 c, which corresponds to an energy of (mean±standard deviation, 3.02±0.06) MeV. After going through the entire accelerator, only 125 particles emerge with a speed of (0.801±0.001) c, which corresponds to the energy of (629±4) MeV. A snapshot of the simulation is shown in **Figure 3**, and the results are shown in **Figure 4** and **Figure 5**, where $\beta = \frac{v}{c}$. The distribution of speeds and energies after the first collimator is shaped as a normal distribution, which was expected, as the particles have only been filtered out by the direction of their velocities. The asymmetry in the speed and energy distributions after the second collimator also makes sense, and it can be attributed to the fact that only the particles close to the test particle speed were properly accelerated, while the rest start lagging behind, even if initially they were faster than the test particle.



Figure 3. 10,000 protons passing through the accelerator.





The loss of most of the particles through the simulation is the result of using only collimators as a means of focusing the beam, instead of using oscillating magnetic fields.

Figure 4. The distribution of particle speeds and energies after passing through the first collimator in the simulation with 10,000 protons. 952 protons passed through the first collimator.



2nd collimator

Figure 5. The distribution of particle speeds and energies after passing through the second collimator in the simulation with 10,000 protons. 952 protons passed through the second collimator.



Simulation with ²⁰⁸Pb⁵³⁺ ions

The following simulation uses the same initial conditions as the last one, except ²⁰⁸Pb⁵³⁺ ions are now accelerated instead of protons.

By letting the test particle through, the change in its speed agrees with the analytic solution from eq. 10. The test particle was accelerated from 0.07989 c to 0.523 c. The distance between the centers of the first two cavities is 119 cm, while the distance between the last two is 317 cm. Considering eq. 9, it can be seen that the final velocity at the end of each cavity depends on the ratio $\frac{|q|}{m}$, which is four times smaller in this simulation than in the previous one, so it is expected that these lead ions are accelerated less than the protons, which consequentially makes the accelerator's cavities longer.

After successfully constructing the accelerator, a particle beam of 10,000 ²⁰⁸Pb⁵³⁺ ions goes through the accelerator. Overall, 1011 particles emerged from the first collimator with an average speed of 0.0800c and a standard deviation of 0.0008 c, which is identical to the previous result, but in this case, it corresponds to the energy of 620±10 MeV due to the ions larger mass. After going through the entire accelerator, only 121 particles with a speed of 0.523±0.004 c emerge from the second collimator, which corresponds to 33.5±0.6 GeV (**Figure 6** and **Figure 7**). The speed and energy distributions are again symmetrical after the first collimator and asymmetrical after the second one, just as in the previous case.



Figure 6. The distribution of particle speeds and energies after passing through the first collimator in the simulation with 10,000 208Pb53+ ions. 1011 ions passed through the first collimator.



Figure 7. The distribution of particle speeds and energies after passing through the second collimator in the simulation with 10,000 208Pb53+ ions. 121 ions passed through the second collimator.

Simulating the DTL part of CERN's Linac4 accelerator with H⁻ ions

CERN's Linac4 accelerator uses an Alvarez-type DTL for part of its acceleration, with which it accelerates hydrogen ions from 0.08 c to 0.31 c (from 3 MeV to 50 MeV) through 120 drift tubes by using the source frequency of 352 MHz [3, 9]. The distances between the centers of neighboring cavities vary from 68 mm to 264 mm [3].

In this simulation, setting $V_{\text{max}} = 300$ kV gives results very similar to the real accelerator as it accelerates particles from ≈ 0.08 c to ≈ 0.31 c. The test particle and the accelerator construction were successfully done. The change in the test particle's speed coincides with eq. 10, and it was accelerated from 0.07 c to 0.31 c with the distances between the centers of neighboring cavities varying from 76 mm to 264 mm which is very close to the real accelerator.

This example is more difficult to simulate with the algorithm used, as the accelerator is much longer, so many particles are lost, which means the initial conditions have to be readjusted so that the beam is more focused. In this simulation, the mean speed of the particles was set to 0.08 c with a standard deviation 1000 times less than the mean; the maximum polar angle was set to just 1°. The first and the final collimator are both 1m long, with a radius of just 1 mm.

After the construction of the Linac4 accelerator, the simulation starts with 10,000 hydrogen ions. Overall, 604 particles pass through the first collimator with a speed of (0.08000 ± 0.00008) c, which corresponds to (2.995 ± 0.006) MeV. At the end of the simulation, only 45 particles got through the second collimator with a speed of (0.26 ± 0.07) c and an energy of (40 ± 20) MeV. A snapshot from the simulation is shown in **Figure 8**, and the histograms with the results are shown in **Figure 9** and **Figure 10**.



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Figure 8. Snapshot from the simulation of the DTL part of CERN's Linac4 accelerator with 10,000 H- ions.



Figure 9. The distribution of particle speeds and energies after passing through the first collimator in the simulation with 10,000 H- ions. 604 ions passed through the first collimator.





Figure 10. The distribution of particle speeds and energies after passing through the second collimator in the simulation with 10,000 H- ions. 45 ions passed through the second collimator.

Analyzing the histograms (**Figure 10**), we can observe that the results are actually better than previously estimated, if looking at just the average values.

Most of the particles that went through the second collimator actually achieved speeds of around 0.31 c, as they should have. The remaining particles were suboptimally accelerated many times, so they significantly lowered the average value. This was to be expected, as this accelerator was much larger than the previous ones.

This example has shown how, with a relatively simple algorithm, it is still possible to get meaningful results when simulating a linac. The biggest problem here was that the particle beam was not focused, which led to the loss of most particles. In reality, the DTL part of CERN's Linac4 accelerator already receives a focused beam of particles that were accelerated in the previous part of the accelerator, and the beam is held focused by using quadrupole magnets.

Discussion

We demonstrated how a linear particle accelerator can be simulated even with a simple algorithm. This is in line with the analytic predictions of eq. 10, and the algorithm itself is very flexible because it can be easily used on any charged particle. All simulations analyzed here give the expected distributions of speeds and energies. By comparing the results from this algorithm to the actual CERN Linac4 accelerator [9], we showed that this algorithm can be used for simulating real accelerators with a certain degree of accuracy, rather than only simple accelerator models.



With a few simple modifications, the algorithm could be further improved. Firstly, the shape of the electric field inside the cavities could be modified. Here we made the simplest assumption that the potential inside the cavities is linear and used it to compare the results with an analytic solution. In real-world applications, one would start from Maxwell's equations and the boundary conditions inside the cavities, but a significant improvement could be achieved just by approximating the standing waves in the RF cavities by a sine function. Furthermore, quadrupole magnets could be introduced to focus the beam. The loss of a large portion of the initial particles is impractical and could damage the device if it were done in practice. In fact, the loss of particles in a real experimental setting is expected to be even larger without quadropole magnets than in this study, as we assumed that the particles inside the beam do not repel each other to make the algorithm simpler and faster to run. The entire code is available on GitHub (github.com/rbarac1/Bachelor-s-Thesis), and the algorithm can be easily modified by changing the electric and magnetic fields into some arbitrary functions.

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