

# Notes on Vacuum Electronics Molecular Dynamics Simulations

Kristinn Torfason

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# 1 Verlet Integration

$$\mathbf{x}_{n+1} = 2\mathbf{x}_n - \mathbf{x}_{n-1} + \frac{\mathbf{F}_n(\mathbf{x}_n)}{m} \Delta t^2 \quad (1)$$

Force on a particle at  $\mathbf{r}$  due to all other particles at positions  $\mathbf{r}_i$

$$\mathbf{F}(\mathbf{r}) = \frac{q^2}{4\pi\epsilon_0} \sum_{i=1}^N \frac{\mathbf{r} - \mathbf{r}_i}{|\mathbf{r} - \mathbf{r}_i|^3} \quad (2)$$

Force on a particle due to an electric field drgdrterter

$$F(\mathbf{r}) = qE(\mathbf{r}) \quad (3)$$

in case of a constant field in the  $z$ -direction  $\mathbf{E} = [0, 0, E_z]$

$$F_z = qE_z = q \frac{V}{d}, \quad (4)$$

where  $V$  is the voltage and  $d$  the gap distance. Initial fictitious previous position

$$x_{n-1} = x_n - v_0 \Delta t - \frac{F(x_n)}{2m} \Delta t^2 \quad (5)$$

where  $v_0$  is the initial velocity.

## 1.1 Velocity Verlet

The Velocity Verlet method is done in three steps, fyrst update the position,

$$x_{n+1} = x_n + v_n \Delta t + \frac{1}{2} a_n \Delta t^2, \quad (6)$$

then calculate the acceleration  $a_{n+1}$  using  $x_{n+1}$  and finally update the velocity,

$$v_{n+1} = v_n + \frac{a_n + a_{n+1}}{2} \Delta t. \quad (7)$$

Note this method assumes that  $a_{n+1}$  dose not depend on  $v_{n+1}$ . This could be a problem when using a magnetic field which depends on the velocity. First approximation would be to use  $v_n$  if the field is week, see also [4].

### 1.1.1 Nondimensionalization

Set  $x_n = L\bar{x}_n$ , where  $L$  is a characteristics length scale and  $\bar{x}_n$  is a dimensionless length. Similarly set  $v_n = T\bar{v}_n$  where  $T$  is a characteristics time scale for the system. Then  $\Delta t = T\bar{\Delta t}$  and  $a_n = \frac{L}{T^2}\bar{a}_n$ . The equations then become,

$$\bar{x}_{n+1} = \bar{x}_n + \bar{v}_n \bar{\Delta t} + \frac{1}{2} \bar{a}_n \bar{\Delta t}^2, \quad (8)$$

and,

$$\bar{v}_{n+1} = \bar{v}_n + \frac{\bar{a}_n + \bar{a}_{n+1}}{2} \bar{\Delta t}. \quad (9)$$

In program  $L = 1.0 * 10^{-9}$  m and  $T = 1.0 * 10^{-12}$  s, i.e. lengths are scaled in nano-meters and time in pico-seconds.

For the Coulomb force we have,

$$F_1 = \frac{q_1 q_2}{4\pi\epsilon} \frac{x_1 - x_2}{|x_1 - x_2|^3}. \quad (10)$$

Setting  $x = L\bar{x}$  gives

$$F_1 = \frac{q_1 q_2}{4\pi\epsilon} \frac{1}{L^2} \frac{\bar{x}_1 - \bar{x}_2}{|\bar{x}_1 - \bar{x}_2|^3}. \quad (11)$$

We wish to find the acceleration using  $F = ma = m \frac{L}{T^2} \bar{a}$  or

$$\bar{a}_1 = \frac{q_1 q_2}{4\pi m \epsilon} \frac{T^2}{L^3} \frac{\bar{x}_1 - \bar{x}_2}{|\bar{x}_1 - \bar{x}_2|^3}. \quad (12)$$

The acceleration from the electric field in the system is given by,

$$F = qE = q \frac{V}{d}, \quad (13)$$

where  $d$  is the gap spacing and  $V$  the voltage over the gap. We set  $d = L\bar{d}$  and  $F = m \frac{L}{T^2}$  and obtain,

$$\bar{a} = \frac{qV}{m\bar{d}} \frac{T^2}{L^2}. \quad (14)$$

## 1.2 Unit Test Case

Two electrons and one hole.

Fyrst electron:  $x_1 = 3$  nm,  $y_1 = -10$  nm,  $z_1 = 101$  nm.

Second electron:  $x_2 = -9$  nm,  $y_2 = 26$  nm,  $z_2 = 80$  nm.

The hole:  $x_3 = 6$  nm,  $y_3 = -24$  nm,  $z_3 = 118$  nm.

Parameters:  $d = 100$  nm,  $V = 2$  V,  $\Delta t = 0.25$  ps.

The acceleration of the fyrst electron is

$$\mathbf{a}_{12} = \frac{e^2}{4\pi m \epsilon_0} \frac{\mathbf{R}_1 - \mathbf{R}_2}{|\mathbf{R}_1 - \mathbf{R}_2|^3} \quad (15)$$

$$\mathbf{a}_{13} = -\frac{e^2}{4\pi m \epsilon_0} \frac{\mathbf{R}_1 - \mathbf{R}_3}{|\mathbf{R}_1 - \mathbf{R}_3|^3} \quad (16)$$

## 2 Field Emission

### 2.1 Fowler-Nordheim equation

$$J = \frac{a}{\phi t^2(l)} F^2 \exp(-\nu(l) b \phi^{3/2} / F) \quad (17)$$

where  $a \approx 1.541434 \times 10^{-6} \text{ AeV}^2$  and  $b \approx 6.830890 \text{ eV}^{-3/2} \text{ Vnm}^{-1}$  are the first and second Fowler-Nordheim constants (see equation (22) and (23)).

The equation for  $\nu(l)$  is [1]

$$\nu(l) = 1 - l + \frac{1}{6} l \ln(l) \quad (18)$$

and for  $t(l)$

$$t(l) = 1 + l \left( \frac{1}{9} - \frac{1}{18} \ln(l) \right) \quad (19)$$

where

$$l = \frac{F}{F_\phi} = \frac{e^3}{4\pi\epsilon_0} \frac{F}{\phi^2} \quad (20)$$

If  $\phi$  is in eV and  $F$  in V/m then

$$l = \frac{e}{4\pi\epsilon_0} \frac{F}{\phi^2} \quad (21)$$

The first Fowler-Nordheim constant is in SI units

$$a_{FN} = \frac{e^3}{8\pi h} \quad (22)$$

and has units  $\text{AJV}^{-2}$ . If we convert to  $\text{AeV}^2$  then we must multiply with  $1/e$  to obtain

$$a_{FN} = \frac{e^2}{8\pi h} = \frac{e^2}{16\pi^2 \hbar} \quad (23)$$

The second Fowler-Nordheim constant is in SI units

$$b_{FN} = \frac{8\pi}{3eh} \sqrt{2m_e} \quad (24)$$

and has the units  $\text{J}^{-3/2} \text{Vm}^{-1}$ . If we convert it to  $\text{eV}^{-3/2} \text{Vm}^{-1}$  then we must multiply it with a factor of  $(1/e)^{-3/2}$  and obtain

$$b_{FN} = \frac{8\pi \sqrt{2m_e} e}{3h} = \frac{4}{3\hbar} \sqrt{2em_e} \quad (25)$$

### 2.2 Surface Field Calculations

If we assume a box with height  $d$  in  $z$ , length  $L$  in  $x$  and  $y$ , with a charge density  $\sigma(z)$ . Then the surface field at the middle of the bottom in the  $z$  direction is given by

$$E = E_0 + 2 \int_0^d \int_{-\frac{L}{2}}^{\frac{L}{2}} \int_{-\frac{L}{2}}^{\frac{L}{2}} \frac{1}{4\pi\epsilon_0} \frac{z\sigma(z)}{(x^2 + y^2 + z^2)^{3/2}} dx dy dz. \quad (26)$$

The factor of two before the integral is to account for image charge effects. If all lengths are scaled with the gap spacing  $d$ ,  $\hat{x} = x/d$ ,  $\hat{y} = y/d$  and  $\hat{z} = z/d$ . Charge density scaled with  $\sigma_0 = 4\pi V_0 \epsilon_0 / d^2$ , which leads to that current density is scaled by the Child Langmuire limit  $\hat{J} = J/J_{CL}$ , or  $\hat{\sigma}(\hat{z}) = \hat{J}/9\pi\sqrt{\hat{z}}$ . The field is scaled by the vacuum field  $E_0 = -V_0/d$ , we then obtain

$$E = 1 - \frac{2J}{9\pi} \int_0^1 \int_{-\frac{L}{2d}}^{\frac{L}{2d}} \int_{-\frac{L}{2d}}^{\frac{L}{2d}} \frac{\sqrt{\hat{z}}}{(\hat{x}^2 + \hat{y}^2 + \hat{z}^2)^{3/2}} d\hat{x} d\hat{y} d\hat{z}. \quad (27)$$

Calculated iteratively

### 2.3 Prolate spheroidal coordinates

The prolate spheroidal coordinates are defined as

$$\begin{aligned} x &= a \sinh \mu \sin \nu \cos \phi \\ y &= a \sinh \mu \sin \nu \sin \phi \\ z &= a \cosh \mu \cos \nu \end{aligned} \quad (28)$$

Set  $\xi = \cosh \mu$  and  $\eta = \cos \nu$  then

$$\begin{aligned} \sinh^2 \mu &= \cosh^2 \mu - 1 = \xi^2 - 1 \\ \sin^2 \nu &= 1 - \cos^2 \nu = 1 - \eta^2 \end{aligned} \quad (29)$$

which gives

$$\begin{aligned} x &= a \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2} \cos \phi \\ y &= a \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2} \sin \phi \\ z &= a \xi \eta \end{aligned} \quad (30)$$

The reverse are

$$\begin{aligned} \xi &= \frac{1}{2a} \left( \sqrt{x^2 + y^2 + (z+a)^2} + \sqrt{x^2 + y^2 + (z-a)^2} \right) \\ \eta &= \frac{1}{2a} \left( \sqrt{x^2 + y^2 + (z+a)^2} - \sqrt{x^2 + y^2 + (z-a)^2} \right) \\ \phi &= \arctan \frac{y}{x} \end{aligned} \quad (31)$$

To find  $\xi$  or  $z$  if given  $x$  and  $y$

$$\xi = \frac{1}{a\sqrt{1-\eta^2}} \sqrt{x^2 + y^2 + a^2(1-\eta^2)} \quad (32)$$

$$z = \frac{\eta}{\sqrt{1-\eta^2}} \sqrt{x^2 + y^2 + a^2(1-\eta^2)} \quad (33)$$

Derivatives of the coordinates

$$\begin{aligned}
\frac{\partial x}{\partial \xi} &= a\xi \frac{\sqrt{1-\eta^2}}{\sqrt{\xi^2-1}} \cos \phi, & \frac{\partial y}{\partial \xi} &= a\xi \frac{\sqrt{1-\eta^2}}{\sqrt{\xi^2-1}} \sin \phi, & \frac{\partial z}{\partial \xi} &= a\eta, \\
\frac{\partial x}{\partial \eta} &= -a\eta \frac{\sqrt{\xi^2-1}}{\sqrt{1-\eta^2}} \cos \phi, & \frac{\partial y}{\partial \eta} &= -a\eta \frac{\sqrt{\xi^2-1}}{\sqrt{1-\eta^2}} \sin \phi, & \frac{\partial z}{\partial \eta} &= a\xi, \\
\frac{\partial x}{\partial \phi} &= -a\sqrt{\xi^2-1}\sqrt{1-\eta^2} \sin \phi, & \frac{\partial y}{\partial \phi} &= a\sqrt{\xi^2-1}\sqrt{1-\eta^2} \cos \phi, & \frac{\partial z}{\partial \phi} &= 0.
\end{aligned} \tag{34}$$

The gradient is

$$\begin{aligned}
\nabla V(\xi, \eta, \phi) &= \hat{x} \frac{\partial V}{\partial \xi} + \hat{y} \frac{\partial V}{\partial \eta} + \hat{z} \frac{\partial V}{\partial \phi} \\
&= \hat{x} \left( \frac{\partial V}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial V}{\partial \eta} \frac{\partial \eta}{\partial x} + \frac{\partial V}{\partial \phi} \frac{\partial \phi}{\partial x} \right) \\
&+ \hat{y} \left( \frac{\partial V}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial V}{\partial \eta} \frac{\partial \eta}{\partial y} + \frac{\partial V}{\partial \phi} \frac{\partial \phi}{\partial y} \right) \\
&+ \hat{z} \left( \frac{\partial V}{\partial \xi} \frac{\partial \xi}{\partial z} + \frac{\partial V}{\partial \eta} \frac{\partial \eta}{\partial z} + \frac{\partial V}{\partial \phi} \frac{\partial \phi}{\partial z} \right)
\end{aligned} \tag{35}$$

The position vector is

$$\vec{r} = \begin{pmatrix} a\sqrt{(\xi^2-1)(1-\eta^2)} \cos \phi \\ a\sqrt{(\xi^2-1)(1-\eta^2)} \sin \phi \\ a\xi\eta \end{pmatrix}, \tag{36}$$

and the unit vector are then

$$\hat{\xi} = \frac{\frac{d\vec{r}}{d\xi}}{\left| \frac{d\vec{r}}{d\xi} \right|}, \quad \hat{\eta} = \frac{\frac{d\vec{r}}{d\eta}}{\left| \frac{d\vec{r}}{d\eta} \right|}, \quad \hat{\phi} = \frac{\frac{d\vec{r}}{d\phi}}{\left| \frac{d\vec{r}}{d\phi} \right|}. \tag{37}$$

For  $\hat{\eta}$  we have

$$\hat{\eta} = \sqrt{\frac{1-\eta^2}{\xi^2-\eta^2}} \begin{pmatrix} -\eta \sqrt{\frac{\xi^2-1}{1-\eta^2}} \cos \phi \\ -\eta \sqrt{\frac{\xi^2-1}{1-\eta^2}} \sin \phi \\ \xi \end{pmatrix} \tag{38}$$

Scale factors are

$$h_\xi = a\sqrt{\frac{\xi^2-\eta^2}{\xi^2-1}}, \quad h_\eta = a\sqrt{\frac{\xi^2-\eta^2}{1-\eta^2}}, \quad h_\phi = a\sqrt{(\xi^2-1)(1-\eta^2)} \tag{39}$$

Given  $x, y$  and  $\eta_1$

$$\xi = \frac{1}{a} \frac{1}{\sqrt{1-\eta_1^2}} \sqrt{x^2 + y^2 + a^2(1-\eta_1^2)} \tag{40}$$

### 2.3.1 Electric Field for Hyperboloid Tip

The vector potential is [2]

$$V(\eta) = V_0 \frac{\ln \left[ \frac{1+\eta_1}{1-\eta_1} \frac{1-\eta}{1+\eta} \right]}{\ln \left[ \frac{1+\eta_1}{1-\eta_1} \frac{1-\eta_2}{1+\eta_2} \right]}. \quad (41)$$

The boundary conditions have been swapped from Ref. [2]. The tip is now held at  $V = 0$  and the anode at  $V = V_0$ . The derivative of the potential is

$$\frac{dV(\eta)}{d\eta} = -\frac{2V_0}{1-\eta^2} \ln^{-1} \left[ \frac{1+\eta_1}{1-\eta_1} \frac{1-\eta_2}{1+\eta_2} \right] \quad (42)$$

The gradient in Prolate-Spheroidal coordinates is

$$\nabla V(\eta) = \frac{1}{a} \sqrt{\frac{1-\eta^2}{\xi^2-\eta^2}} \frac{dV(\eta)}{d\eta} \hat{\eta}, \quad (43)$$

and the electric field is

$$\vec{E} = -\nabla V(\eta) = \frac{2V_0}{a} \frac{1}{\xi^2-\eta^2} \frac{1}{\ln \left[ \frac{1+\eta_1}{1-\eta_1} \frac{1-\eta_2}{1+\eta_2} \right]} \begin{pmatrix} -\eta \sqrt{\frac{\xi^2-1}{1-\eta^2}} \cos \phi \\ -\eta \sqrt{\frac{\xi^2-1}{1-\eta^2}} \sin \phi \\ \xi \end{pmatrix} \quad (44)$$

Here  $\xi$ ,  $\eta$  and  $\phi$  are the position inside the diode. While  $\eta_1$  is the hyperboloid tip and  $\eta_2 = 0$  is the anode plane.

$$|\vec{E}| = \frac{2V_0}{a} \frac{1}{\sqrt{\xi^2-\eta^2} \sqrt{1-\eta^2}} \frac{1}{\ln \left[ \frac{1+\eta_1}{1-\eta_1} \frac{1-\eta_2}{1+\eta_2} \right]} \quad (45)$$

At the top of the tip we have  $\eta = \eta_1$  and  $\xi = 1$  and the electric field points in the  $z$ -direction,

$$E_z = \frac{2V_0}{a} \frac{1}{1-\eta_1^2} \frac{1}{\ln \left[ \frac{1+\eta_1}{1-\eta_1} \right]}. \quad (46)$$

### 2.3.2 Area Calculations for Hyperboloid Tip

The Surface area is given by the integral

$$A = \int_{\xi_1}^{\xi_2} \int_{\phi_1}^{\phi_2} h_\xi h_\phi d\xi d\phi. \quad (47)$$

Where  $h_\xi$  and  $h_\phi$  are the scale factors.

$$A = a^2 \sqrt{1-\eta^2} (\phi_2 - \phi_1) \int_{\xi_1}^{\xi_2} \sqrt{\xi^2 - \eta^2} d\xi \quad (48)$$

The integral can be found in Ref. [3, eq. 2.271-3]. The results are

$$A = \frac{a^2}{2} \sqrt{1-\eta^2} (\phi_2 - \phi_1) \left[ \xi \sqrt{\xi^2 - \eta^2} - \eta^2 \ln \left( \xi + \sqrt{\xi^2 - \eta^2} \right) \right]_{\xi_1}^{\xi_2} \quad (49)$$

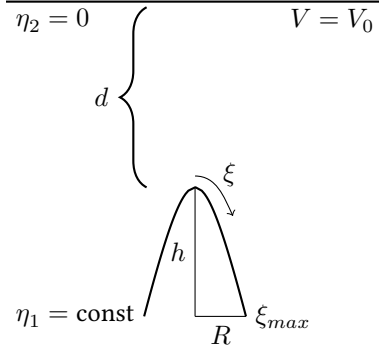


Figure 1: Coordinates

### 2.3.3 Arc length

To find the arc length use

$$\begin{aligned} x &= a \sinh \mu \sin \nu \cos \phi \\ y &= a \sinh \mu \sin \nu \sin \phi \\ z &= a \cosh \mu \cos \nu \end{aligned} \quad (50)$$

$$\begin{aligned} \frac{\partial x}{\partial \mu} &= a \cosh \mu \sin \nu \cos \phi \\ \frac{\partial y}{\partial \mu} &= a \cosh \mu \sin \nu \sin \phi \\ \frac{\partial z}{\partial \mu} &= a \sinh \mu \cos \nu \end{aligned} \quad (51)$$

$$\begin{aligned} \left( \frac{\partial x}{\partial \mu} \right)^2 + \left( \frac{\partial y}{\partial \mu} \right)^2 + \left( \frac{\partial z}{\partial \mu} \right)^2 &= a^2 (\cosh^2 \mu \sin^2 \nu + \sinh^2 \mu \cos^2 \nu) \\ &= \sin^2 \nu + \sinh^2 \mu \\ &= \cosh^2 \mu - \cos^2 \nu \end{aligned} \quad (52)$$

$$S = \int_0^{\mu_\ell} \sqrt{\sin^2 \nu + \sinh^2 \mu} \, d\mu \quad (53)$$

### 2.3.4 Fixed Tip Size

Define the base radius  $R$  and height of the tip  $h$  from the base (See Figure 1). We then have

$$R = a \sqrt{\xi_{max}^2 - 1} \sqrt{1 - \eta_1^2} \quad (54)$$

$$h = -a \xi_{max} \eta_1 - d = -(d + a \xi_{max} \eta_1) \quad (55)$$

and also

$$\eta_1 = -\frac{d}{a} \quad (56)$$



By inserting Equation (56) into Equation (55) we get

$$\xi_{max} = \frac{h}{d} + 1 \quad (57)$$

We can then use Equation (57) and Equation (54) to obtain

$$a = \sqrt{\frac{d^2 R^2}{h^2 + 2dh} + d^2} \quad (58)$$

It is possible to use Equations (56), (57) and (56) to keep the shape of the tip constant for all  $d$ .

### 2.3.5 Radius of Curvature

Radius of Curvature is

$$R = \left| \frac{\left( \left( \frac{dx}{d\xi} \right)^2 + \left( \frac{dz}{d\xi} \right)^2 \right)^{\frac{3}{2}}}{\frac{dx}{d\xi} \frac{d^2 z}{d\xi^2} - \frac{dz}{d\xi} \frac{d^2 x}{d\xi^2}} \right|. \quad (59)$$

Set  $\phi = 0$  and  $\eta = \eta_1$ , we then have

$$\frac{d^2 x}{d\xi^2} = -a \frac{\sqrt{1 - \eta_1^2}}{(\xi^2 - 1)^{\frac{3}{2}}} \quad (60)$$

and

$$\frac{d^2 z}{d\xi^2} = 0. \quad (61)$$

Therefore,

$$R = \left| \frac{a (\xi^2 - \eta_1^2)^{\frac{3}{2}}}{\eta_1 \sqrt{1 - \eta_1^2}} \right|. \quad (62)$$

If  $\xi = 1$  and  $\eta_1 = -\frac{a}{d}$  then

$$R = \frac{a^2}{d} - d. \quad (63)$$

### 2.3.6 Normal Vector to Surface

Starting with

$$\xi = \frac{1}{2a} \left( \sqrt{x^2 + y^2 + (z+a)^2} + \sqrt{x^2 + y^2 + (z-a)^2} \right) \quad (64)$$

and inserting this into

$$z = a\xi\eta = \frac{\eta}{2} \left( \sqrt{x^2 + y^2 + (z+a)^2} + \sqrt{x^2 + y^2 + (z-a)^2} \right). \quad (65)$$

Now solve for  $z$  to obtain

$$z = f(x, y) = \frac{\pm\eta}{\sqrt{1-\eta^2}} \sqrt{x^2 + y^2 + a(1-\eta^2)}. \quad (66)$$

The normal vector the point  $(x_0, y_0)$  is then

$$\vec{N} = [f_x(x_0, y_0), f_y(x_0, y_0), -1], \quad (67)$$

or

$$\vec{N} = \left[ \frac{\eta}{\sqrt{1-\eta^2}} \frac{x_0}{\sqrt{x_0^2 + y_0^2 + a^2(1-\eta^2)}}, \frac{\eta}{\sqrt{1-\eta^2}} \frac{y_0}{\sqrt{x_0^2 + y_0^2 + a^2(1-\eta^2)}}, -1 \right]. \quad (68)$$

This vector points into the surface. Its norm is

$$|\vec{N}|^2 = \frac{1}{1-\eta^2} - \frac{a^2\eta}{x_0^2 + y_0^2 + a^2(1-\eta^2)}. \quad (69)$$

### 2.3.7 Spherical Image Charge Approximation

A charged particle a distance  $y$  away from the center of a sphere will have an image charge partner at a distance  $y'$  away from the center of the sphere.

$$y' = \frac{a^2}{y}, \quad (70)$$

where  $a$  is the radius of the sphere. The charge of it will be

$$q' = -\frac{a}{y}q, \quad (71)$$

where  $q$  is the charge of the particle at  $y$ .

### 3 Cylindrical Geometry

#### 3.1 Electric Field

The Laplace equation in cylindrical coordinates is

$$\nabla^2 \Phi = \frac{1}{r} \frac{\delta}{\delta r} \left( r \frac{\delta \Phi}{\delta r} \right) + \frac{1}{r^2} \frac{\delta^2 \Phi}{\delta \theta^2} + \frac{\delta^2 \Phi}{\delta z^2} = 0. \quad (72)$$

Due to symmetry in  $\theta$  and  $z$  we have

$$\Phi = \Phi(r), \quad (73)$$

or

$$\nabla^2 \Phi(r) = \frac{1}{r} \frac{\delta}{\delta r} \left( r \frac{\delta \Phi(r)}{\delta r} \right) = 0. \quad (74)$$

Integration yields,

$$\frac{\delta \Phi(r)}{\delta r} = \frac{A}{r}, \quad (75)$$

where  $A$  is a constant. A second integration then gives,

$$\Phi(r) = A \ln(r) + B, \quad (76)$$

where  $B$  is also a constant. The boundary conditions seen in Fig. 2 are  $\Phi(R_i) = V_0$

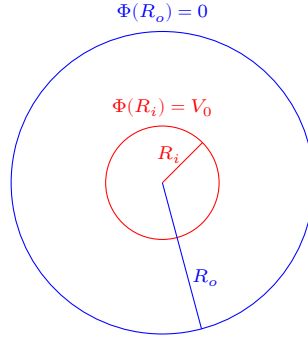


Figure 2: A schematic illustration of the system.

and  $\Phi(R_o) = 0$ . Using them to solve for the constants gives

$$B = V_0 \frac{\ln(R_o)}{\ln(R_o/R_i)}, \quad (77)$$

and

$$A = \frac{V_0}{\ln(R_i/R_o)}. \quad (78)$$

The electric field is then

$$\vec{E} = -\vec{\nabla} \Phi = - \left( \frac{\delta \Phi}{\delta r} \hat{r} + \frac{1}{r} \frac{\delta \Phi}{\delta \theta} \hat{\theta} + \frac{\delta \Phi}{\delta z} \hat{z} \right), \quad (79)$$

or

$$\vec{E} = \frac{V_0}{\ln(R_o/R_i)} \frac{\hat{r}}{r} = \frac{V_0}{\ln(R_o/R_i)} \frac{\cos(\theta)\hat{x} + \sin(\theta)\hat{y}}{r}. \quad (80)$$

### 3.2 Emission

The emission process checks the angle between the position vector (black solid line) and the acceleration (violet dashed line) (see Fig. 3). If the angle  $\theta$  is greater than  $\pi/2$  then emission can occur.

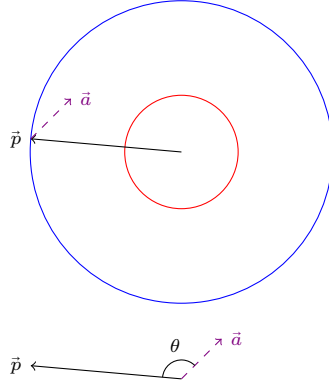


Figure 3: Angle between position and acceleration.

## 4 Circuit elements

### 4.1 Series with Resistor and Capacitor

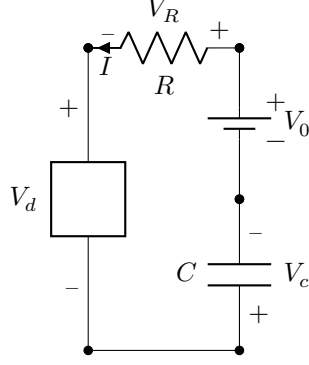


Figure 4: Circuit

For the circuit we have

$$V_0 = V_d + V_R + V_c \quad (81)$$

or

$$V_c(t) = V_0 - V_d - IR. \quad (82)$$

For the capacitor

$$I(t) = C \frac{dV_c(t)}{dt} = C \left[ \frac{dV_0(t)}{dt} - \frac{dV_d(t)}{dt} - R \frac{dI(t)}{dt} \right], \quad (83)$$

or

$$-C \frac{dV_d(t)}{dt} = RC \frac{dI(t)}{dt} + I(t), \quad (84)$$

note that  $V_0$  is constant in time. Integration from 0 to  $t$  yields,

$$V_d(t) = V_d(0) + R[I(0) - I(t)] - \frac{1}{C} \int_0^t I(\tau) d\tau. \quad (85)$$

The initial conditions  $V_d(0) = V_0$  and  $I(0) = 0$  give,

$$V_d(t) = V_0 - RI(t) - \frac{1}{C} \int_0^t I(\tau) d\tau. \quad (86)$$

The numerical integration can be done using the trapezoidal rule,

$$\int_{t_n}^{t_{n+1}} I(\tau) d\tau \approx \Delta t \frac{I(t_n) + I(t_{n+1})}{2}, \quad (87)$$

or

$$\int_0^{t_{n+1}} I(\tau) d\tau = \int_0^{t_n} I(\tau) d\tau + \int_{t_n}^{t_{n+1}} I(\tau) d\tau = \int_0^{t_n} I(\tau) d\tau + \Delta t \frac{I(t_n) + I(t_{n+1})}{2}, \quad (88)$$

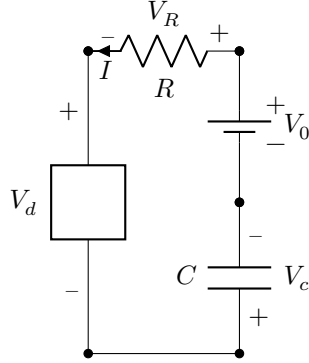


Figure 5: Todo change this figure

## 4.2 Parallel Capacitor

For this circuit we have

$$I = I_d + I_C, \quad (89)$$

$$V_d = V_{RC} + V_C, \quad (90)$$

$$V_d = V_s - V_R, \quad (91)$$

$$I_C = C \frac{dV_C}{dt}, \quad (92)$$

$$V_{RC} = R_C I_C, \quad (93)$$

$$V_R = RI. \quad (94)$$

The goal is to write  $V_d$  as a function of  $I_d$ .

$$V_d = V_s - V_R = V_s - RI = V_s - R(I_d + I_C) = V_s - RI_d - RC \frac{dV_C}{dt}. \quad (95)$$

We now get rid of  $V_C$  by setting  $V_C = V_d - V_{RC}$  to obtain,

$$V_d = V_s - RI_d - RC \frac{dV_d}{dt} + RC \frac{V_{RC}}{dt}. \quad (96)$$

Rewriting the equation and using the  $V_{RC} = R_C C \frac{dV_C}{dt}$  gives,

$$RC \frac{dV_d}{dt} + V_d = V_s - RI_d + RC \frac{V_{RC}}{dt} = V_s - RI_d + RR_C C^2 \frac{d^2 V_C}{dt^2}. \quad (97)$$

We again end up with  $V_C$  in our equation. To get rid of it we use equation 95,

$$RC \frac{dV_C}{dt} = V_s - RI_d - V_d, \quad (98)$$

then taking the derivative and multiplying with  $R_C C$ ,

$$RR_C C^2 \frac{d^2 V_C}{dt^2} = -RR_C C \frac{dI_d}{dt} - R_C C \frac{dV_d}{dt}. \quad (99)$$

We then obtain,

$$RC \frac{dV_d}{dt} + V_d = V_s - RI_d - RR_C C \frac{dI_d}{dt} - R_C C \frac{dV_d}{dt}, \quad (100)$$

or rearranging terms,

$$(R + R_C)C \frac{dV_d}{dt} + V_d = V_s - RI_d - RR_C C \frac{dI_d}{dt}. \quad (101)$$

This is a linear differential equation,  $\frac{dV_d(t)}{dt} + f(t)V_d(t) = g(t)$ , with a general solution given by,

$$V_d(t) = e^{-\int f(t) dt} \left( \int g(t) e^{\int f(t) dt} dt + \kappa \right), \quad (102)$$

where  $\kappa$  is a constant determined by the initial conditions  $V_d(0) = V_s$ ,  $f(t) = \frac{1}{C(R+R_C)}$  and  $g(t) = \frac{1}{C(R+R_C)} (V_s + RI_d - RR_C C \frac{dI_d}{dt})$ . Let's set  $b = C(R + R_C)$ , then  $\int_0^t f(t') dt' = \frac{t}{b}$ . Integration of the terms in  $g(t)$  yeilds,

$$\int_0^t V_s e^{t'/b} dt' = bV_s (e^{t/b} - 1), \quad (103)$$

$$\int_0^t \frac{dI_d}{dt'} e^{t'/b} dt' = [e^{t'/b} I_d]_0^t - \frac{1}{b} \int_0^t I_d e^{t'/b} dt' = I_d e^{t/b} I_d(0) - \frac{1}{b} \int_0^t I_d e^{t'/b} dt'. \quad (104)$$

The solutions the becomes,

$$V_d(t) = \frac{1}{b} e^{-t/b} \left[ bV_s (e^{t/b} - 1) - R \int_0^t I_d e^{t'/b} dt' - RR_C C \left( I_d e^{t/b} - I_d(0) - \frac{1}{b} \int_0^t I_d e^{t'/b} dt' \right) + \kappa \right], \quad (105)$$

or

$$V_d(t) = \frac{1}{b} e^{-t/b} \left[ bV_s (e^{t/b} - 1) - \left( R - \frac{RR_C C}{b} \right) \int_0^t I_d e^{t'/b} dt' - RR_C C (I_d e^{t/b} - I_d(0)) + \kappa \right]. \quad (106)$$

Using the initial conditions  $V_d(0) = V_s$  and  $I_d(0) = 0$  gives  $\kappa = bV_s$ ,

$$V_d(t) = e^{-t/b} \left[ V_s e^{t/b} - \frac{1}{b} \left( R - \frac{RR_C C}{b} \right) \int_0^t I_d e^{t'/b} dt' - \frac{RR_C C}{b} I_d e^{t/b} \right]. \quad (107)$$

In the end we get

$$V_d(t) = V_s - \frac{R^2}{(R + R_C)^2 C} \int_0^t I_d(t') e^{\frac{t'-t}{C(R+R_C)}} dt' - \frac{RR_C}{R + R_C} I_d(t). \quad (108)$$

For the numerical integration we have

$$\int_{t_n}^{t_{n+1}} I(t') e^{\frac{t'-t_{n+1}}{C(R+R_C)}} dt' = \frac{\Delta t}{2} \left( I(t_n) e^{-\frac{\Delta t}{C(R+R_C)}} + I(t_{n+1}) \right). \quad (109)$$

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