Notes on Vacuum Electronics Molecular Dynamics Simulations

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April 20, 2018

1 Verlet Integration

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

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

$$\mathbf{F}(\mathbf{r}) = \frac{q^2}{4\pi\varepsilon_0}\sum_{i=1}^{N}\frac{\mathbf{r}-\mathbf{r}_i}{|\mathbf{r}-\mathbf{r}_i|^3} \tag{2}$$

Force on a particle due to an electric field drgdrterter

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

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

$$F_z = qE_z = q\frac{V}{d}, \tag{4}$$

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

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

where v_0 is the initial velocity.

1.1 Velocity Verlet

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

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

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

$$v_{n+1} = v_n\frac{a_n + a_{n+1}}{2}\Delta t^2\,. \tag{7}$$

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 $\Delta t = T\Delta\bar{t}$ and $a_n = \frac{L}{T^2}\bar{a}_n$. The equations then become,

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

and,

$$\bar{v}_{n+1} = \bar{v}_n\frac{\bar{a}_n + \bar{a}_{n+1}}{2}\Delta\bar{t}^2\,. \tag{9}$$

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

For the Coulomb force we have,

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

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

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

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

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

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

$$F = qE = q\frac{V}{d} \,, \tag{13}$$

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,

$$\bar{a} = \frac{qV}{m\bar{d}} \frac{T^2}{L^2} \,. \tag{14}$$

1.2 Unit Test Case

Two electrons and one hole.
Fyrst electron: $x_1 = 3\,\mathrm{nm}$, $y_1 = -10\,\mathrm{nm}$, $z_1 = 101\,\mathrm{nm}$.
Second electron: $x_2 = -9\,\mathrm{nm}$, $y_2 = 26\,\mathrm{nm}$, $z_2 = 80\,\mathrm{nm}$.
The hole: $x_3 = 6\,\mathrm{nm}$, $y_3 = -24\,\mathrm{nm}$, $z_3 = 118\,\mathrm{nm}$.
Parameters: $d = 100\,\mathrm{nm}$, $V = 2\,\mathrm{V}$, $\Delta t = 0.25\,\mathrm{ps}$.

The acceleration of the fyrst electron is

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

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

2 Field Emission

2.1 Fowler-Nordheim equation

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

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

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

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

and for $t(l)$

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

where

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

If ϕ is in eV and F in V/m then

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

The first Fowler-Nordheim constant is in SI units

$$a_{FN} = \frac{e^3}{8\pi h} \tag{22}$$

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

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

The second Fowler-Nordheim constant is in SI units

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

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

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

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

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

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

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

Calculated iteratively

2.3 Prolate spheroidal coordinates

The prolate spheroidal coordinates are defined as

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

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

$$\begin{aligned} sinh^2\, \mu = cosh^2\, \mu - 1 = \xi^2 - 1 \\ sin^2\, \nu = 1 - cos^2\, \nu = 1 - \eta^2 \end{aligned} \tag{29}$$

which gives

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

The reverse are

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

To find ξ or z if given x and y

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

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

Derivatives of the coordinates

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

The gradient is

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

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

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

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 η_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 Hyperbolid Tip

The vector potential is [2]

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

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

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

The gradient in Prolate-Spherodial coordinates is

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

and the electric field is

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

Here ξ, η and ϕ are the position inside the diode. While η_1 is the hyberbolid tip and $\eta_2 = 0$ is the anode plane.

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

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

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

2.3.2 Area Calculations for Hyperbolid Tip

The Surface area is given by the integral

$$A = \int_{\xi_1}^{\xi_2}\int_{\phi_1}^{\phi_2} h_\xi h_\phi\, \mathrm{d}\xi\mathrm{d}\phi\,. \tag{47}$$

Where h_ξ and h_ϕ are the scale factors.

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

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

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

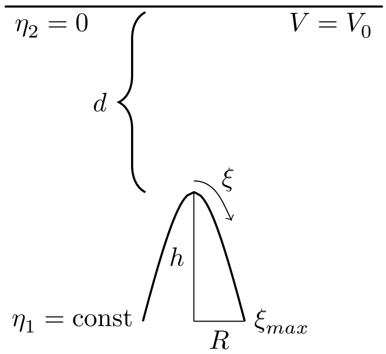

Figure 1: Coordinates

2.3.3 Arc length

To find the arc length use

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

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

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

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

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

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

$$h = -a\xi_{max}\eta - d = -\left(d + a\xi_{max}\eta_1\right) \tag{55}$$

and also

$$\eta_1 = -\frac{d}{a} \tag{56}$$

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

$$\xi_{max} = \frac{h}{d} + 1 \tag{57}$$

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

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

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

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

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

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

and

$$\frac{\mathrm{d}^2 z}{\mathrm{d}\xi^2} = 0 . \tag{61}$$

Therefore,

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

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

$$R = \frac{a^2}{d} - d . \tag{63}$$

2.3.6 Normal Vector to Surface

Starting with

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

and inserting this into

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

Now solve for z to obtain

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

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

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

or

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

This vector points into the surface. Its norm is

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

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.

$$y' = \frac{a^2}{y}, \tag{70}$$

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

$$q' = -\frac{a}{y} q, \tag{71}$$

where q is the charge of the particle at y.

3 Cylindrical Geometry

3.1 Electric Field

The Laplace equation in cylindrical coordinates is

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

Due to symmetry in θ and z we have

$$\Phi = \Phi(r)\,, \tag{73}$$

or

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

Integration yields,

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

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

$$\Phi(r) = A\,ln(r) + B\,, \tag{76}$$

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

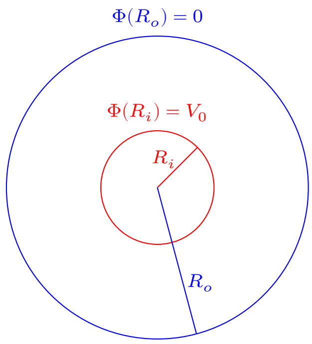

Figure 2: A schematic illustration of the system.

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

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

and

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

The electric field is then

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

or

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

3.2 Emission

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

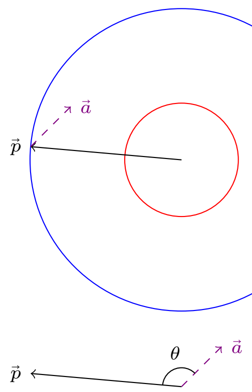

Figure 3: Angle between position and acceleration.

4 Circuit elements

4.1 Series with Resistor and Capacitor

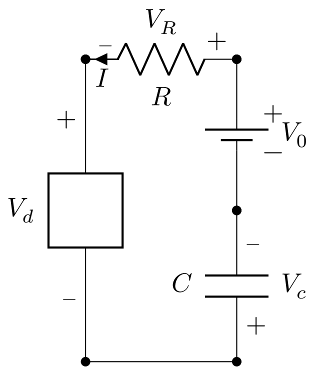

Figure 4: Circuit

For the circuit we have

$$V_0 = V_d + V_R + V_c \tag{81}$$

or

$$V_c(t) = V_0 - V_d - IR\,. \tag{82}$$

For the capacitor

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

or

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

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

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

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

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

The numberical integration can be done using the trapezoidal rule,

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

or

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

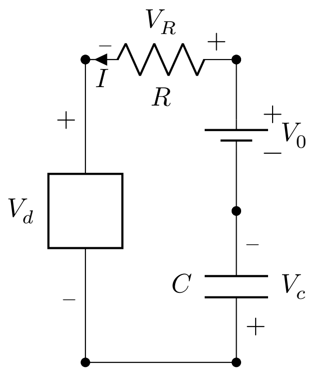

Figure 5: Todo change this figure

4.2 Parallel Capacitor

For this circuit we have

$$I = I_d + I_C \,, \tag{89}$$
$$V_d = V_{RC} + V_C \,, \tag{90}$$
$$V_d = V_s - V_R \,, \tag{91}$$
$$I_C = C\frac{dV_C}{dt} \,, \tag{92}$$
$$V_{RC} = R_C I_C \,, \tag{93}$$
$$V_R = RI \,. \tag{94}$$

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

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

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

$$V_d = V_s - RI_d - RC\frac{dV_d}{dt} + RC\frac{V_{RC}}{dt} \,. \tag{96}$$

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

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

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

$$RC\frac{dV_C}{dt} = V_s - RI_d - V_d \,, \tag{98}$$

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

$$RR_C C^2\frac{d^2V_C}{dt^2} = -RR_C C\frac{dI_d}{dt} - R_C C\frac{dV_d}{dt} \,. \tag{99}$$

We then obtain,

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

or rearranging terms,

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

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

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

where κ is a constant determined by the initial conditions $V_d(0)=V_s$, $f(t)=\frac{1}{C(R+R_C)}$ and $g(t)=\frac{1}{C(R+R_C)}\left(V_s+RI_d-RR_CC\frac{dI_d}{dt}\right)$. 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,

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

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

The solutions the becomes,

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

or

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

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

$$V_d(t)=e^{-t/b}\left[V_se^{t/b}-\frac{1}{b}\left(R-\frac{RR_CC}{b}\right)\int_0^t I_de^{t'/b}dt'-\frac{RR_CC}{b}I_de^{t/b}\right]\,. \tag{107}$$

In the end we get

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

For the numerical integration we have

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

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