# S-BASED MACRO-PARTICLE SPECTRAL ALGORITHM FOR AN ELECTRON GUN 

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#### Abstract

We derive a Hamiltonian description of a continuous particle distribution and its electrostatic potential from the Low Lagrangian. The self consistent space charge potential is discretized according to the spectral Galerkin approximation. The particle distribution is discretized using macro-particles. We choose a set of initial and boundary conditions to model the TRIUMF 300keV thermionic DC electron gun. The field modes and macro-particle coordinates are integrated selfconsistently. The current status of the implementation is discussed.


## INTRODUCTION

The section of beamline we are trying to model includes the electron gun (Fig. 1) and one solenoid, a total length of 57 cm up to the first view screen. The electrons are emitted from a hot cathode. An RF grid is placed a fraction of a millimetre downstream from the cathode. It is used to modulate the emission of electrons at 650 MHz . Electrons are accelerated to 300 keV using a DC field. The distance between the cathode and the ground electrode is 12 cm . The emitting surface of the cathode has a radius of 4 mm . The nominal bunch charge is 15 pC with a bunch length of 130 ps , see [1]. The solenoid enables us to adjust the phase advance between the cathode and the view screen. At a particular phase advance, we can use the electron beam to create an image of the RF grid on the view screen see Fig. 2. Scanning the phase advance enables us to measure the transverse phase space distribution using tomography [2]. Our objective is to reproduce these measurements using an algorithm derived from the least action principle like in [3-5]. The description of thermionic emission and effects from the grid are outside the scope of this model.
Following classical field theory conventions, let an over dot ' '. represent an explicit derivative with respect to time, and similarly a prime ' $/$ ' denotes a partial derivative with respect to $z$. We write the vectors that lie in the transverse $x y$ plane with a lower ' $\perp$ '. For example: $\mathbf{x}_{\perp}$ is the vector $(x, y, 0)$.

## CONTINUOUS MODEL

We start from the Low Lagrangian [6] which is a sum of two integrals:

$$
\begin{align*}
L= & \int \mathrm{d}^{3} \mathbf{x}_{0} \mathrm{~d}^{3} \dot{\mathbf{x}}_{0} \mathcal{L}_{p}\left(\mathbf{x}\left(\mathbf{x}_{0}, \dot{\mathbf{x}}_{0}, t\right), \dot{\mathbf{x}}\left(\mathbf{x}_{0}, \dot{\mathbf{x}}_{0}, t\right) ; \mathbf{x}_{0}, \dot{\mathbf{x}}_{0}, t\right)  \tag{1}\\
& +\int \mathrm{d}^{3} \overline{\mathbf{x}} \mathcal{L}_{f}(\phi, \mathbf{A} ; \overline{\mathbf{x}}, t),
\end{align*}
$$



Figure 1: OPERA Model of the 300 keV TRIUMF electron gun with equipotential lines of the electric potential.


Figure 2: The view screen image, after the first solenoid.
where the Lagrangian densities are:

$$
\begin{align*}
& \mathcal{L}_{p}\left(\mathbf{x}, \dot{\mathbf{x}} ; \mathbf{x}_{0}, \dot{\mathbf{x}}_{0}, t\right)= \\
& \quad f\left(\mathbf{x}_{0}, \dot{\mathbf{x}}_{0}\right)\left(-m c^{2} \sqrt{1-|\dot{\mathbf{x}}|^{2} / c^{2}}-q \phi(\mathbf{x}, t)+q \dot{\mathbf{x}} \cdot \mathbf{A}(\mathbf{x}, t)\right), \\
& \mathcal{L}_{f}(\phi, \mathbf{A} ; \mathbf{x}, t)=  \tag{2}\\
& \quad \frac{\epsilon_{0}}{2}\left(|\nabla \phi(\mathbf{x}, t)+\dot{\mathbf{A}}(\mathbf{x}, t)|^{2}-c^{2}|\nabla \times \mathbf{A}(\mathbf{x}, t)|^{2}\right) . \tag{3}
\end{align*}
$$

and $\bar{x}$ is a dummy variable of integration.
To describe the self field we make the assumption that in the centre of mass frame the self field is completely described by the scalar potential $\varphi(\mathbf{x}, t)$, and the vector potential is zero. We assume that the beam is travelling in the positive $z$-direction, with unit vector $\hat{z}$. Now, by applying an active

Lorentz transformation we find that this field corresponds to:

$$
\begin{align*}
& \phi(\mathbf{x}, t)=\gamma_{0} \varphi(\mathbf{x}, t)  \tag{4}\\
& \mathbf{A}(\mathbf{x}, t)=\frac{\beta_{0}}{c} \gamma_{0} \varphi(\mathbf{x}, t) \hat{z}=\frac{\beta_{0}}{c} \phi(\mathbf{x}, t) \hat{z} \tag{5}
\end{align*}
$$

in the laboratory frame. The fields before and after transformation are functions of the coordinates in the laboratory frame. $c \beta_{0}$ is the centre of mass velocity and $\gamma_{0}$ is the corresponding Lorentz factor. We also assume:

$$
\begin{equation*}
\dot{\mathbf{x}} \cdot \hat{z} \approx c \beta_{0} \tag{6}
\end{equation*}
$$

Now, we can write the new Lagrangian densities as:

$$
\begin{align*}
& \mathcal{L}_{p}\left(\mathbf{x}, \dot{\mathbf{x}} ; \mathbf{x}_{0}, \dot{\mathbf{x}}_{0}, t\right)=-f m c^{2} \sqrt{1-|\dot{\mathbf{x}}|^{2} / c^{2}}-f q \gamma_{0}^{-2} \phi(\mathbf{x}, t),  \tag{7}\\
& \mathcal{L}_{f}(\phi ; \overline{\mathbf{x}}, t)= \\
& \quad \frac{\epsilon_{0}}{2}\left(\gamma_{0}^{-2}\left|\nabla_{\perp} \phi(\overline{\mathbf{x}}, t)\right|^{2}+\mid \partial_{\bar{z}} \phi(\overline{\mathbf{x}}, t)+c^{-1} \partial_{t}\left(\left.\beta_{0} \phi(\overline{\mathbf{x}}, t)\right|^{2}\right),\right. \tag{8}
\end{align*}
$$

so we have described the self field using only a scalar potential.

To check the reasonableness of the field Lagrangian we look at the equation of motion for the scalar field which is:

$$
\begin{equation*}
\left(\partial_{z}+\frac{\beta_{0}}{c} \partial_{t}\right)^{2} \phi+\frac{\beta_{0}^{\prime}}{c} \dot{\phi}+\left(1-\beta_{0}^{2}\right) \nabla_{\perp}^{2} \phi=0 \tag{9}
\end{equation*}
$$

In the ultra-relativistic limit $\beta_{0}=1$ we find that the transverse dynamics of $\phi$ become frozen and we have the following equation of motion:

$$
\begin{equation*}
\left(\partial_{z}+\frac{1}{c} \partial_{t}\right)^{2} \phi=0 \tag{10}
\end{equation*}
$$

The solutions to this equation are wave-fronts travelling in the $z$ direction with speed $c$. In the stationary limit $\beta_{0}=0$ we find the Laplace equation:

$$
\begin{equation*}
\phi^{\prime \prime}+\nabla_{\perp}^{2} \phi=0 \tag{11}
\end{equation*}
$$

Thus far we have described a Lagrangian system with two main assumptions, the self-field in the beam frame is electrostatic and that $\Delta \beta / \beta_{0} \ll 1$.

## Change of Independent Variable

Changing the independent variable in the Lagrangian is done using coordinate transformation $[7,8]$. We find that the new Lagrangian density is:

$$
\begin{align*}
& \mathcal{L}_{p}\left(\mathbf{x}_{\perp}, t, \mathbf{x}_{\perp}^{\prime}, t^{\prime} ; z\right)= \\
& \quad-f m c \sqrt{\left(c t^{\prime}\right)^{2}-\left|\mathbf{x}_{\perp}^{\prime}\right|^{2}-1}-f q \gamma_{0}^{-2} t^{\prime} \phi\left(\mathbf{x}_{\perp}, t, z\right) \tag{12}
\end{align*}
$$

and the field Lagrangian density is unchanged.

## Hamiltonian

Since we have taken $z$ as the independent variable, we can take $\gamma_{0}$ and $\beta_{0}$ to be solely functions of $z$. The momentum density canonically conjugated to particle position is:

$$
\begin{gather*}
P_{\mathbf{x}_{\perp}}\left(x_{0}, y_{0}, t_{0}, x_{0}^{\prime}, y_{0}^{\prime}, t_{0}^{\prime}, z\right)=\frac{\partial \mathcal{L}_{p}}{\partial \mathbf{x}_{\perp}^{\prime}} \\
=\frac{f m c \mathbf{x}_{\perp}^{\prime}}{\sqrt{\left(c t^{\prime}\right)^{2}-\left|\mathbf{x}_{\perp}^{\prime}\right|^{2}-1}} \tag{13}
\end{gather*}
$$

$$
\begin{align*}
& -E\left(x_{0}, y_{0}, t_{0}, x_{0}^{\prime}, y_{0}^{\prime}, t_{0}^{\prime}, z\right)=\frac{\partial \mathcal{L}_{p}}{\partial t^{\prime}} \\
& =\frac{-f m c^{3} t^{\prime}}{\sqrt{\left(c t^{\prime}\right)^{2}-\left|\mathbf{x}_{\perp}^{\prime}\right|^{2}-1}}-f q \gamma_{0}^{-2} \phi \tag{14}
\end{align*}
$$

As for the scalar potential, we have that:

$$
\begin{equation*}
\pi_{\phi}\left(\mathbf{x}_{\perp}, t, z\right)=\frac{\partial \mathcal{L}_{f}}{\partial \phi^{\prime}}=\epsilon_{0}\left(\partial_{z}+\frac{\beta_{0}}{c} \partial_{t}\right) \phi \tag{15}
\end{equation*}
$$

So, we find the Hamiltonian to be:
$H=\int \mathrm{d} x_{0} \mathrm{~d} y_{0} \mathrm{~d} t_{0} \mathrm{~d} x_{0}^{\prime} \mathrm{d} y_{0}^{\prime} \mathrm{d} t_{0}^{\prime} \mathcal{H}_{p}\left(\mathbf{x}_{\perp}, t, \mathbf{P}_{\perp}, E ; x_{0}, y_{0}, t_{0}, x_{0}^{\prime}, y_{0}^{\prime}, t_{0}^{\prime}\right)$

$$
\begin{equation*}
+\int \mathrm{d}^{2} \overline{\mathbf{x}}_{\perp} \mathrm{d} \bar{t} \mathcal{H}_{f}\left(\phi, \pi_{\phi} ; \overline{\mathbf{x}}_{\perp}, \bar{t}, z\right) \tag{16}
\end{equation*}
$$

where the Hamiltonian densities are given by the Legendre transform:

$$
\begin{align*}
\mathcal{H}_{p} & =P_{\mathbf{x}_{\perp}} \cdot \mathbf{x}_{\perp}^{\prime}-E t^{\prime}-\mathcal{L}_{p} \\
& =-\sqrt{\frac{1}{c^{2}}\left(E-q f \gamma_{0}^{-2} \phi\left(\mathbf{x}_{\perp}, t, z\right)\right)^{2}-\left|\mathbf{P}_{\perp}\right|^{2}-(m f c)^{2}}  \tag{17}\\
\mathcal{H}_{f} & =\pi_{\phi} \phi^{\prime}-\mathcal{L}_{f}=\frac{\pi_{\phi}^{2}}{2 \epsilon_{0}}-\frac{\beta_{0}}{c} \pi_{\phi} \dot{\phi}-\frac{\epsilon_{0}}{2 \gamma_{0}^{2}}\left(\nabla_{\perp} \phi\right)^{2}
\end{align*}
$$

Lastly, we can examine the equations of motion:

$$
\begin{array}{rlrl}
\mathbf{x}_{\perp}^{\prime} & =\frac{\mathbf{P}_{\perp}}{P_{z}}, & \mathbf{P}_{\perp}^{\prime}=q f \gamma_{0}^{-2} t^{\prime} \nabla_{\perp} \phi\left(\mathbf{x}_{\perp}, t, z\right) \\
t^{\prime} & =\frac{E-q f \gamma_{0}^{-2} \phi\left(\mathbf{x}_{\perp}, t, z\right)}{c^{2} P_{z}}, & E^{\prime} & =q f \gamma_{0}^{-2} t^{\prime} \partial_{t} \phi\left(\mathbf{x}_{\perp}, t, z\right) \tag{19}
\end{array}
$$

where

$$
\begin{equation*}
P_{z}=\sqrt{\frac{1}{c^{2}}\left(E-q f \gamma_{0}^{-2} \phi\left(\mathbf{x}_{\perp}, t, z\right)\right)^{2}-\left|\mathbf{P}_{\perp}\right|^{2}-(m f c)^{2}} \tag{20}
\end{equation*}
$$

as well as the equations of motion for the scalar potential canonical pair:

$$
\begin{equation*}
\phi^{\prime}=\frac{\pi_{\phi}}{\epsilon_{0}}-\frac{\beta_{0}}{c} \dot{\phi}, \quad \pi_{\phi}^{\prime}=\frac{\epsilon_{0}}{\gamma_{0}^{2}} \nabla_{\perp}^{2} \phi+\frac{\beta_{0}}{c} \dot{\phi} \tag{21}
\end{equation*}
$$

These equations of motion are useful to get an intuitive picture of the model. To obtain the discrete Hamiltonian we can now discretize our Lagrangian system and follow the same steps.

## DISCRETEIZATION

Our choice of discretization scheme is:

$$
\begin{equation*}
f\left(\mathbf{x}_{0}, \dot{\mathbf{x}}_{0}\right)=\sum_{j} w^{j} \delta^{(3)}\left(\mathbf{x}_{0}^{j}-\mathbf{x}_{0}\right) \delta^{(3)}\left(\dot{\mathbf{x}}_{0}^{j}-\dot{\mathbf{x}}_{0}\right) \tag{22}
\end{equation*}
$$

$$
\begin{align*}
& \phi(x, y, t, z)= \\
& \sum_{n m \ell} \Phi_{n m \ell}(z) \cos \left(\frac{n \pi x}{L_{x}}\right) \cos \left(\frac{m \pi y}{L_{y}}\right) \cos \left(\frac{\ell \pi \Delta t}{L_{t}}\right) \tag{23}
\end{align*}
$$

where the particle distribution is a sum of Dirac delta functions which gives us point-like model particles. The basis functions of the scalar potential are chosen such that each of
them satisfies the boundary conditions, the Galerkin approximation. The field is contained in the box of size $L_{x} \times L_{y} \times L_{t}$ and is zero at the boundaries. The self field is periodic in time with the period being the RF period, and zero at the boundaries. The field mode labels $n, m, \ell$ are positive odd integers. This selects the modes that satisfy the boundary conditions and are even functions about each axis.
Substituting these into the Lagrangian, simplifying and solving for the Hamiltonian gives:

$$
\begin{equation*}
H=\sum_{j} H^{j}\left(\mathbf{x}_{\perp}^{j}, \mathbf{P}_{\perp}^{j}, t^{j}, E^{j} ; z\right)+\sum_{n m \ell} H_{n m \ell}\left(\Phi_{n m \ell}, \Pi_{n m \ell} ; z\right) \tag{24}
\end{equation*}
$$

where the model particle Hamiltonian for particle $j$ is:

$$
\begin{align*}
H^{j}= & -\sqrt{\frac{1}{c^{2}}\left(P_{t}^{j}-q w^{j} \gamma_{0}^{-2} \phi\left(\mathbf{x}_{\perp}^{j}, t^{j}, z\right)\right)^{2}-\left|\mathbf{P}_{\perp}^{j}\right|^{2}-\left(m w^{j} c\right)^{2}} \\
& -\left(\Delta E^{j}+E_{0}\right) t_{0}^{\prime}+\Delta t^{j} E_{0}^{\prime}, \tag{25}
\end{align*}
$$

and for field mode $n, m, \ell$ it is:

$$
\begin{align*}
& H_{n m \ell}= \\
& \frac{1}{2 V} \Pi_{n m \ell}^{2}-\frac{V}{2 \gamma_{0}^{2}}\left(\left(\frac{n \pi}{L_{x}}\right)^{2}+\left(\frac{m \pi}{L_{y}}\right)^{2}+\left(\frac{\beta_{0} \gamma_{0} \ell \pi}{c L_{t}}\right)^{2}\right) \Phi_{n m \ell}^{2} \tag{26}
\end{align*}
$$

where $V$ is a volume factor given by $V=\frac{1}{8} \epsilon_{0} L_{x} L_{y} L_{t}$. Note that the $\pi_{\phi} \dot{\phi}$ term became decoupled in this Hamiltonian because of the orthogonality of the basis functions and its derivatives. The discretized Hamiltonian yields an equation of motion for each of the discrete degrees of freedom.
The equations of motion for the macro-particles are:

$$
\begin{array}{r}
\mathbf{x}_{\perp}^{j \prime}=\frac{\mathbf{P}_{\perp}^{j}}{P_{z}^{j}}, \quad \Delta t^{j \prime}=\frac{P_{t}^{j}-q w^{j} \gamma_{0}^{-2} \phi\left(\mathbf{x}_{\perp}^{j}, t^{j}, z\right)}{c^{2} P_{z}^{j}}+t_{0}^{\prime} \\
\mathbf{P}_{\perp}^{j \prime}=w^{j} q \gamma_{0}^{-2}\left(t_{0}^{\prime}-\Delta t^{j \prime}\right) \nabla_{\perp} \phi\left(\mathbf{x}_{\perp}^{j}, t^{j}, z\right) \\
\Delta E^{j \prime}=w^{j} q \gamma_{0}^{-2}\left(t_{0}^{\prime}-\Delta t^{j \prime}\right) \dot{\phi}\left(\mathbf{x}_{\perp}^{j}, t^{j}, z\right)-E_{0}^{\prime} \tag{28}
\end{array}
$$

where the longitudinal particle momentum is calculated by:

$$
\begin{equation*}
P_{z}^{j}=-\sqrt{\frac{1}{c^{2}}\left(P_{t}^{j}-q w^{j} \gamma_{0}^{-2} \phi\left(\mathbf{x}_{\perp}^{j}, t^{j}, z\right)\right)^{2}-\left|\mathbf{P}_{\perp}^{j}\right|^{2}-\left(m w^{j} c\right)^{2}} . \tag{29}
\end{equation*}
$$

Also, the equations of motion for the field modes are given by:

$$
\begin{align*}
& \Phi_{n m \ell}^{\prime}=\frac{1}{V} \Pi_{n m \ell} \\
& \Pi_{n m \ell}^{\prime}=\frac{V}{\gamma_{0}^{2}}\left(\left(\frac{n \pi}{L_{x}}\right)^{2}+\left(\frac{m \pi}{L_{y}}\right)^{2}+\left(\frac{\beta_{0} \gamma_{0} \ell \pi}{c L_{t}}\right)^{2}\right) \Phi_{n m \ell} \\
& +\sum_{j} \frac{q w^{j}}{c^{2} \gamma_{0}^{2}}\left(\Delta t^{j^{\prime}}-t_{0}^{\prime}\right) \cos \left(\frac{n \pi x^{j}}{L_{x}}\right) \cos \left(\frac{m \pi y^{j}}{L_{y}}\right) \cos \left(\frac{\ell \pi \Delta t^{j}}{L_{t}}\right), \tag{30}
\end{align*}
$$

## IMPLEMENTATION AND FUTURE WORK

The current implementation is written in Python as vectorized Numpy code. The system of differential equations These equations of motion are a consistent set of coupled first order ordinary differential equations.
is solved using the scipy.integrate module. One integration method is chosen and the equations are integrated simultaneously with appropriate tolerances for adaptive step size methods. All of the integration methods provided by the module were tested and integrating the fields was unconditionally unstable.

Future work is to understand and address the problems with integration.

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