

# Particle in Cell code

Sara Gómez, Universidad EAFIT.

Jaime Humberto Hoyos, Universidad de Medellín.

This Live Script was developed in order to understand the particle-in-cell method. The quantities of the code are not physical since the aim of this document is visualize each step of the method. The code is based on the work of [Giovanni Lapenta](#) from K.U.Leuven.

## Variables

- L: Length of the system.
- dt: Time step.
- Nt: Number of time steps.
- Ng: Grid points.
- WP: Plasma frequency.
- N1: Number of particles.
- V01: Mean velocity.
- Vth1: Thermal velocity.
- QM1: Charge mass relation.
- XP1: Amplitude of the perturbation.
- Mode1: Mode of the perturbation.

The first step is to define the parameters of the code:

```
clear
L = 1;
dt = 0.5;
Nt = 1;
Ng = 6;
WP = 1;
dx = L/(Ng-1);
```

Then we will define the properties beam:

```
N1 = 5;
V01 = 0;
Vth1 = 0.1;
QM1 = -1;
XP1 = 0;
Mode1 = 0;
```

Then we are going to define the charge of the super-particles and the background density:

```
Q1 = (WP^2)/(QM1*N1/L)
```

```
Q1 = -0.2000
```

```
rho_back = -N1*Q1/L
```

```
rho_back = 1
```

Now, the particles will be positioned along the x axis with a sinusoidal perturbation, taking into account that the code is one-dimensional.

```
time = 0:dt:(Nt-1)*dt;  
space = linspace(0,L,Ng);  
xp1 = (linspace(0,L-L/N1,N1))'
```

```
xp1 = 5×1  
      0  
      0.2000  
      0.4000  
      0.6000  
      0.8000
```

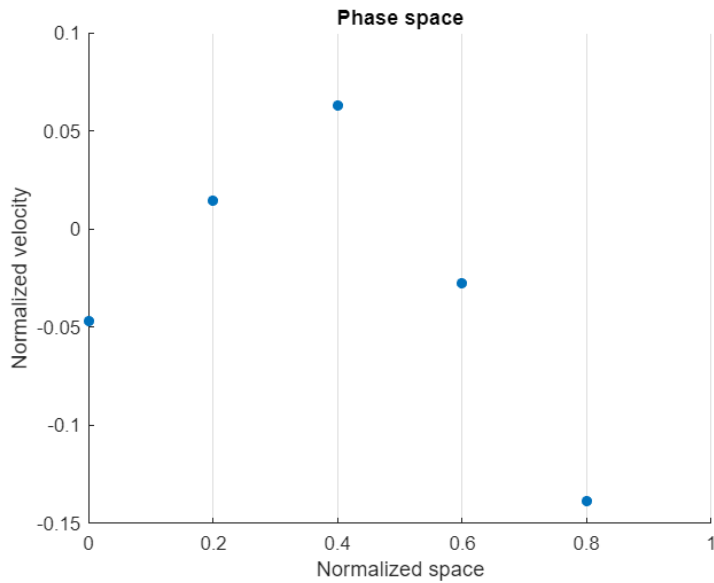
```
xp1 = xp1 + XP1*(L/N1)*sin(2*pi*xp1/L*Mode1);
```

Then, we will give a velocity to the beam. In first place we multiply the thermal velocity with the function `randn(NS,1)` which returns an NS-by-1 matrix of normally distributed random numbers.

```
vp1 = Vth1*randn(N1,1);  
vp1 = vp1 + V01
```

```
vp1 = 5×1  
     -0.0467  
      0.0145  
      0.0631  
     -0.0277  
     -0.1385
```

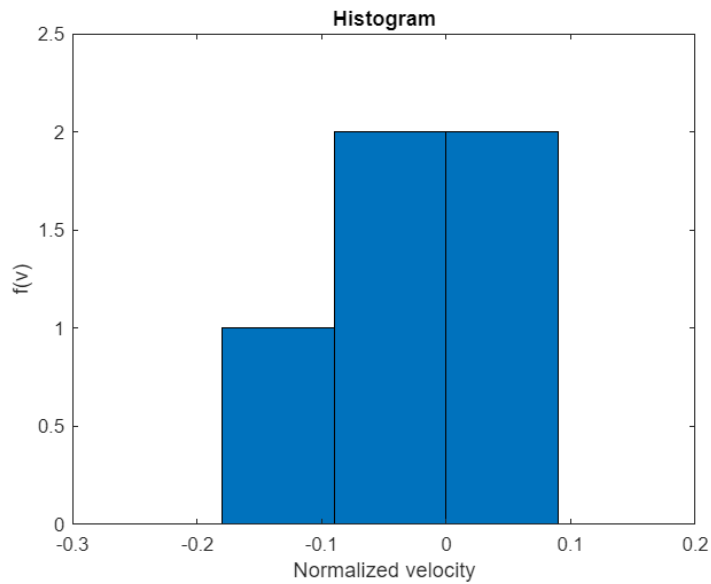
```
figure;  
scatter(xp1,vp1,30,'filled')  
title('Phase space')  
xlabel('Normalized space')  
ylabel('Normalized velocity')  
xlim([0 L])  
xticks(space)  
ax = gca;  
ax.XGrid = 'on';
```



```
ax.YGrid = 'off';
```

We can plot the histogram in order to see how particles are distributed.

```
histfit([vp1])
title('Histogram')
xlabel('Normalized velocity')
ylabel('f(v)')
```



One way to taste the functionality of the code is to see the energy and the momentum conservation. Momentum is defined as:

$$P = \sum_p m_p v_p$$

The kinetic energy is:

$$E_k = \frac{1}{2} \sum_p m_p v_p^2$$

and the potential energy is:

$$E_p = \frac{1}{2} \epsilon_0 \sum_g (E_g^2) dx$$

where  $E_g$  is the field in the grid points.

Then we will prepare the vectors for momentum, kinetic energy and potential energy as:

```
mom = zeros(1, Nt); E_kin = zeros(1, Nt); E_pot = zeros(1, Nt);
```

In order to find the electric field, we need to solve the Poisson's equation which is define as:

$$\nabla^2 \phi = \frac{\rho}{\epsilon_0}$$

where  $\phi$  is the electric potential. The Poisson's equation can be discretized in 1D using the classic three point formula:

$$\epsilon_0 \frac{\phi_{g+1} - 2\phi_g + \phi_{g-1}}{dx^2} = -\rho_g$$

In this way we need to define a matrix with the coefficients that multiply  $\phi$  wich will be  $A_x$ .

$$A_x \Phi = -\rho_g dx^2$$

```
Phi = 0;
un = ones(Ng-1, 1);
Ax = spdiags([un -2*un un], [-1 0 1], Ng-1, Ng-1);
```

Then we observe the form of the matrix  $A_x$ :

```
full(Ax)
```

```
ans = 5x5
    -2     1     0     0     0
     1    -2     1     0     0
     0     1    -2     1     0
     0     0     1    -2     1
     0     0     0     1    -2
```

The variable `mat1` is the interpolation function and `p1` is an auxiliary vector. We will explain later this variables.

```
mat1 = 0; Eg = 0;
p1 = 1:N1; p1 = [p1 p1];
```

## Computational Cycle

Now we are going to star with the comutational cycle

```
for it = 1:Nt
```

## Diagnostics

In first place we will find out the momentum and the energy for each iteration

```
mom(it) = (Q1)*(sum(vp1));  
E_kin(it) = 0.5*abs(Q1)*(sum(vp1.^2));  
E_pot(it) = 0.5*sum(Eg.^2)*dx;
```

## Newton's equations: Updating the positions

Then we will update positions. By Newton's equations we have:

$$\frac{dx_p}{dt} = v_p$$

$$\frac{dv_p}{dt} = \frac{q_s}{m_s} E_p$$

The Euler method will be used to discretize the equations:

$$x_p^{n+1} = x_p^n + \Delta t v_p^{n+1}$$

$$v_p^{n+1} = v_p^n + \Delta t \frac{q_s}{m_s} E_p^{n+1}$$

Then we have:

```
xp1 = xp1 + vp1*dt
```

```
xp1 = 5x1  
-0.0234  
0.2073  
0.4316  
0.5862  
0.7307
```

## Periodic boundary conditions

Now, applying the periodic boundary conditions:

- If xp1 is less than 0, then add L to the xp1 position.
- If xp1 is greater or equal than L, then subtract L to the xp1 position.

```
out1 = (xp1<0); xp1(out1) = xp1(out1) + L;  
out1 = (xp1>=L); xp1(out1) = xp1(out1) - L;
```

Then, we will save the values of the velocities and the electric field for each iteration:

## Projection

Now we will project the properties of the particles to the grid.

For doing this we will introduce the function `floor` which rounds each element to the nearest integer less than or equal to that element. We will save that information in a vector called `Project_1 = [i_1 ; i1_1]`.

```
xp1
```

```
xp1 = 5×1
    0.9766
    0.2073
    0.4316
    0.5862
    0.7307
```

```
i_1 = floor(xp1/dx)+1
```

```
i_1 = 5×1
     5
     2
     3
     3
     4
```

```
i1_1 = i_1 + 1
```

```
i1_1 = 5×1
     6
     3
     4
     4
     5
```

```
Project_1 = [i_1 ; i1_1];
```

## Fraction

Now we want to compute what fraction of the particle size lies on the two nearest grid points using:

```
Fi_1 = abs((xp1/dx) - i_1 )
```

```
Fi_1 = 5×1
    0.1168
    0.9637
    0.8422
    0.0692
    0.3463
```

```
Fi1_1 = 1 - Fi_1
```

```
Fi1_1 = 5×1
    0.8832
    0.0363
    0.1578
    0.9308
    0.6537
```

```
Fraction_1 = [Fi_1;Fi1_1];
```

Then we will apply the boundary conditions on the projections:

- If the projection is less than 1, then add Ng.
- If the projection is greater than Ng, then subtract Ng.

```
out = (lt(Project_1,1)); Project_1(out) = Project_1(out)+Ng;
out = (gt(Project_1,Ng));Project_1(out) = Project_1(out)-Ng;
Project_1
```

```
Project_1 = 10x1
    5
    2
    3
    3
    4
    6
    3
    4
    4
    5
```

## Interpolation matrix

The matrix `mat` is the interpolation function. This will allow us to carry the information between super-particles and the grid. We will use the auxiliary vectors in order to build this matrix. The vectors are defined as `p1 = 1:N1`; `p1 = [p1 p1]`. Below is the vector `p1`.

`p1`

```
p1 = 1x10
    1    2    3    4    5    1    2    3    4    5
```

Then we will define a Interpolation matrix of size `Ns*Ng`, where it writes the fraction of the particles in the position (`p1,Project_1`). The index of the matrix `p1` will give us the information of the particle, while the index `Project_1` will give us the information of the grid point.

```
mat1 = sparse(p1, Project_1, Fraction_1, N1, Ng);
full(mat1)
```

```
ans = 5x6
    0         0         0         0    0.1168    0.8832
    0    0.9637    0.0363         0         0         0
    0         0    0.8422    0.1578         0         0
    0         0    0.0692    0.9308         0         0
    0         0         0    0.3463    0.6537         0
```

```
sum(full(mat1'))
```

```
ans = 1x5
    1    1    1    1    1
```

## Charge density

Now, we need to find the charge density in the nodes of the grid. By definition:

$$\rho = \sum_s \frac{Q_s}{dx}.$$

```
rho1 = full((Q1/dx)*sum(mat1))';
rhot = rho1 + rho_back;
```

## Computing Electric Field

Let us remember the Poisson's equation:

$$\epsilon_0 \frac{\phi_{g+1} - 2\phi_g + \phi_{g-1}}{dx^2} = -\rho_g$$

$$A_x \Phi = -\rho_g dx^2$$

For solving this equation we will use the backslash (\) operator.

```
Phi=Ax\(-rhot(1:Ng-1)*dx^2);
Phi=[Phi;0]
```

```
Phi = 6x1
    0.0311
    0.0222
    0.0118
   -0.0007
    0.0042
         0
```

Now, for solving the electric field we need to discretize the following equation:

$$E = -\frac{d\phi}{dx}.$$

The electric field is computed in the grid points from the discrete potentials as:

$$E_g = -\frac{\phi_{g+1} - \phi_{g-1}}{2dx}.$$

In first place we define  $\phi_{g-1}$ :

```
Phi
```

```
Phi = 6x1
    0.0311
    0.0222
    0.0118
   -0.0007
    0.0042
         0
```

```
Phim1 = [Phi(Ng); Phi(1:Ng-1)]
```

```
Phim1 = 6x1
         0
    0.0311
    0.0222
    0.0118
```



```
-0.0007  
0.0042
```

Then, we define  $\phi_{g+1}$ :

```
Phip1 = [Phi(2:Ng); Phi(1)]
```

```
Phip1 = 6×1  
0.0222  
0.0118  
-0.0007  
0.0042  
0  
0.0311
```

Finally, we compute the electric field:

```
Eg = -(Phip1 - Phim1)/(2*dx)
```

```
Eg = 6×1  
-0.0554  
0.0482  
0.0571  
0.0188  
-0.0017  
-0.0671
```

### Move particles:

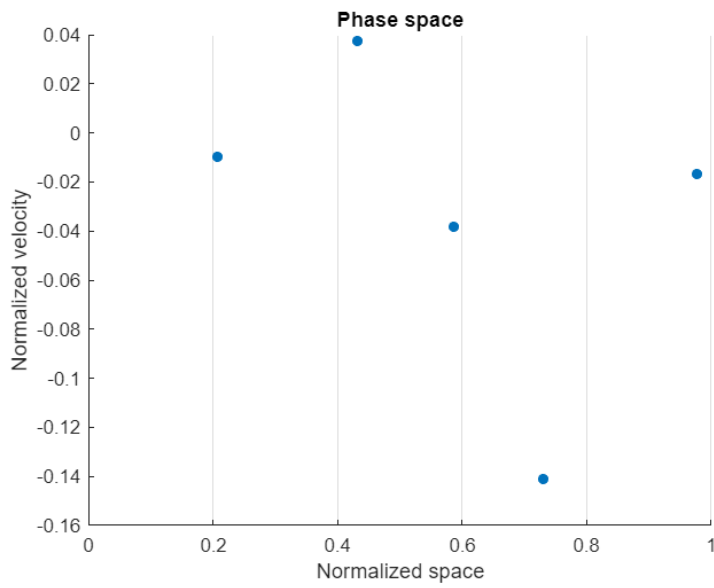
Applying the Euler method for moving the particles:

```
vp1 = vp1 + QM1*mat1*Eg*dt
```

```
vp1 = 5×1  
-0.0170  
-0.0097  
0.0376  
-0.0384  
-0.1412
```

Finally, can see the Phase space of the system.

```
scatter(xp1, vp1, 30, 'filled')
```



```
title('Phase space')
xlabel('Normalized space')
ylabel('Normalized velocity')
xlim([0 L])
xticks(space)
ax = gca;
ax.XGrid = 'on';
end
```