MATHEMATICAL DESCRIPTION OF THE DENSITY PROFILE FOR THE INTERACTION OF AN ULTRA-HIGH INTENSITY LASER PULSE WITH A NANOSTRUCTURED FLAT-TOP CONE

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The density profile of the plasma created by an ultra-high intensity laser pulse interacting with a new nanostructured flat-top cone target is described mathematically. The walls and the top of the nanostructured flat-top cone are coated with a layer of nanospheres which have the same diameter and are tangent to each other. This density profile is useful in two-dimensional Particle-in-Cell simulations for laser-ion acceleration.

Keywords: nanostructured flat-top cone, density profile, ultra-high intensity laser pulse, nanospheres.

1. Introduction

In the last two decades, a lot of target geometries were proposed in order to obtain very energetic protons which can be used to treat cancer [1–6]. Several papers showed that the interaction of the ultra-high intensity laser pulse with a micro-cone target can generate protons accelerated at energies of tens of MeV with low angular divergence and high laser absorption [7–11] in the Target Normal Sheath Acceleration and Direct laser-light-pressure regimes. Other works were devoted to different kinds of cone targets suitable for proton acceleration at energies up to few tens of MeV [12–17] or high-power laser pulse intensification [18]. We proposed in a previous article a plastic flat-top cone with a nanostructured foil in the top, named as 'cone with nanospheres' [19]. In the case of the interaction of a circularly polarized ultra-high intensity laser pulse with a flat-top cone and a cone with nanospheres we obtained more energetic protons and carbon ions for the cone with nanospheres. These results motivated us to improve this cone target.

We propose a new nanostructured cone target. It is a flat-top cone with the walls and the top coated inside with nanospheres. These nanospheres have the same diameter and are tangent to the walls as well as to each other. We depict

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mathematically the density profile of the initial plasma created by an ultra-high intensity laser pulse interacting with a nanostructured flat-top cone. This density profile is designed to be used in two-dimensional Particle-in-Cell (PIC) codes.

This paper is organized as follows. In Section 2, we describe the nanostructured flat-top cone inside a simulation box. In Section 3, we obtain the formula for the number of nanospheres from the top of the cone and the formula for the number of nanospheres on the walls of the cone. In Section 4, we find the conditions for a charged particle associated with a mathematical point to be inside or outside of a nanosphere (from the walls or the top of the cone). We conclude with some remarks.

2. Parameters of a nanostructured flat-top cone inside a simulation box

Particle-in-Cell (PIC) simulation codes need an initial density profile of the initial plasma created at the interaction of an ultra-high intensity laser pulse with a target. The density profile corresponds to the geometry shape of the target, in our case a nanostructured flat-top cone. This cone has curved walls. PIC simulations are performed by inserting the target in a simulation box. In Figure 1 we sketch a two-dimensional nanostructured flat-top cone geometry inside a simulation box.

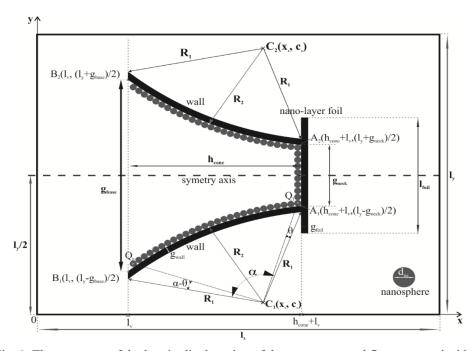


Fig. 1. The geometry of the longitudinal section of the nanostructured flat-top cone inside a simulation box.

The nanostructured flat-top cone parameters are relative to a Cartesian coordinate system whose origin O is the left down corner of the simulation box. The x- and y-axis are the two perpendicular sides of the simulation box which intersect at the point O. The target has a conical shape with curved walls. Both walls have a given thickness, g_{wall} . The walls are circular arcs of the circles with the radii R_1 and $R_2=R_1+g_{wall}$, with the centers $C_1(x_1,c_1)$ and $C_2(x_2,c_2=l_y-c_1)$, respectively. There is a foil on the top with the thickness g_{foil} and width l_{foil} . The other geometric parameters of the nanostructured cone are: the height h_{cone} , the large base of the cone g_{base} and the small base of the cone g_{neck} (Figure 1). The walls and the top are coated inside with nanospheres as can be seen in Figure 1. All nanospheres have the same diameter d_{ns} and are tangent to each other. The nanostructured cone is inserted in a simulation box with the width l_x and the height l_y . In the PIC simulations one must consider a vacuum before the target. We denote the vacuum width as l_{ν} .

We have also the following notations in Figure 1: $B_{1(2)}$ are the interior points of the intersection of the cone base with the bottom (upper) wall of the cone and $A_{I(2)}$ are the interior points of the intersection of the top of the cone with the bottom (upper) wall of the cone.

In Figures 2(a) and 2(b) is drawn the arrangement of the nanospheres on the walls and top of the cone, respectively.

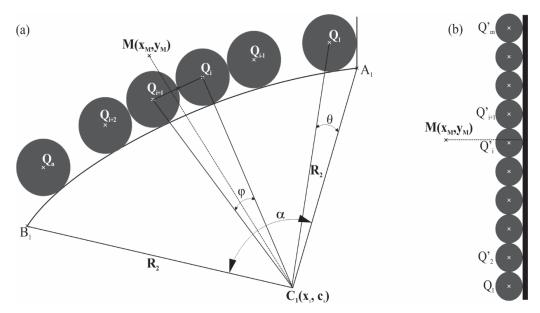


Fig. 2. (a) The enlarged scale geometry of the bottom wall of the nanostructured flat-top cone and the mathematical point associated with a charged particle $M(x_M, y_M)$; (b) The enlarged scale geometry of the cone top.

The mathematical notations and quantities from the Figures 2(a) and 2(b) which will be used in our formulas are:

 Q_I - the center of the first nanosphere tangent to the top of the cone and to the arc A_1B_1 ;

 Q_n - the center of the last nanosphere tangent to the arc A_1B_1 , closest to the base of the cone, where n is the total number of nanospheres tangent to the cone wall;

 Q'_m - the center of the last nanosphere tangent to the top of the cone and to the arc A_2B_2 , where m is the total number of nanospheres tangent to the cone top.

 $M(x_M, y_M)$ - a mathematical point associated with a charged particle (electron, proton or ion)

$$\theta \stackrel{\text{def}}{=} m(\widehat{Q_1C_1A_1}), \ \alpha \stackrel{\text{def}}{=} m(\widehat{B_1C_1A_1}) \Rightarrow m(\widehat{B_1C_1Q_1}) = \alpha - \theta$$

$$\varphi \stackrel{\text{def}}{=} m(\widehat{Q_{i+1}C_1Q_i}), \text{ where } i = \overline{1, n-1}.$$

We consider the following variables as being known: h_{cone} , g_{base} , g_{neck} , g_{foil} , l_{foil} , l_{v} , l_{x} , l_{y} , d_{ns} and c_{1} .

We notice that we have a high enough number of nanospheres tangent to the walls of the cone, such that the angles θ and φ are smaller than $\pi/2$. All the centers of the *n* nanospheres on a cone wall, $Q_1, ..., Q_n$, are on a circle with the center C_1 and the radius $R_2+d_{ns}/2$.

The configuration from above describes mathematically the density profile used in the PIC simulations of the interaction of an ultra-high intensity laser pulse with a nanostructured cone target.

3. The number of nanospheres

To be able to describe the density profile for the nanostructured cone it is necessary to know how many nanospheres can coat the walls on the inside. For this propose, we need to find the abscissa of the circle center $C_I(x_I, c_I)$ and the other quantities depending on the known values.

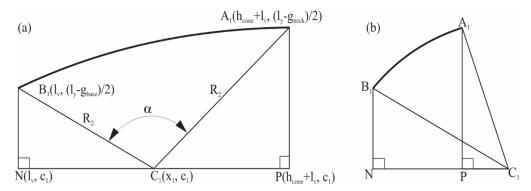


Fig. 3. Two possible cases of the position of the circle center C_l : (a) $x_1 < h_{cone} + l_v$; (b) $x_1 \ge h_{cone} + l_v$.

Due to the fact that the arc A_1B_1 is a part of the circle with the center C_1 and the target is a cone trunk with a small base A_1A_2 and a large base B_1B_2 , as can be seen in Figure 1, the point C_I can be located between the points A_I and B_I (case (a)) or in front of the point A_I (case (b)), as can be seen in Figure 3. In order to find the abscissa of the circle center C_I , we must calculate the lengths of the segments NC_I , B_1N , C_1P and A_1P (Figure 3). It is straightforward to evaluate them as following:

(a) For $x_1 < h_{cone} + l_v$ we have

$$NC_1 = x_1 - l_v \tag{1}$$

$$NC_1 = x_1 - l_v$$

$$B_1 N = \frac{l_y - g_{base}}{2} - c_1$$
(1)

$$C_1 P = h_{cone} + l_v - x_1 \tag{3}$$

$$C_{1}P = h_{cone} + l_{v} - x_{1}$$

$$A_{1}P = \frac{l_{y} - g_{neck}}{2} - c_{1}$$
(3)

(b) For $x_1 \ge h_{cone} + l_v$, NC_1 , B_1N , A_1P have the same dimensions as in case (a) and

$$C_1 P = x_1 - (h_{cone} + l_v) \tag{5}$$

Due to the fact that $B_1C_1=A_1C_1=R_2$ the radius of the circle with the center $C_1(x_1,c_1)$ and using the Pythagorean Theorem in the right-angle triangles ΔB_1NC_1 and $\Delta A_1 PC_1$ we obtain the formula for the abscissa x_1

$$x_1 = \frac{(l_y - 2c_1 - g_{nb})g_{bn}}{2h_{cone}} + \frac{h_{cone} + 2l_v}{2},$$
where $g_{nb} = \frac{g_{base} + g_{neck}}{2}$, $g_{bn} = \frac{g_{base} - g_{neck}}{2}$ (6)

But m is the number of the nanospheres from the top of the con, i. e. an integer number, therefore we have

$$m = \left[\frac{g_{neck}}{d_{ns}}\right] \tag{7}$$

Also, n is the number of nanospheres tangent to one of the inside walls of the cone. It is straightforward to determine the inequalities

$$(n-1) \cdot \varphi < \alpha \text{ and } \theta + n\varphi \ge \alpha, \text{ with } \theta, \varphi \in (0,\pi/2)$$
 (8)

We obtain from the relations (8) the condition which the number n must fulfill

$$\frac{\alpha - \theta}{\varphi} \le n < \frac{\alpha - \theta}{\varphi} + 1 \tag{9}$$

From the relation (9) and due to the fact that n is an integer number, n must be the integer part of the ratio $(\alpha-\theta)/\phi$

$$n = \left[\frac{\alpha - \theta}{\varphi}\right] \tag{10}$$

In order to determine the number of nanospheres on the cone walls, n we have to find the quantities α , φ and θ .

As a consequence of the condition $\alpha \in (0, \pi)$, the cos function is bijective and thus the inverse $arccos \alpha$ is uniquely determined. We apply the generalized Pythagorean Theorem in the triangle $\Delta A_1 B_1 C_1$ and we get

$$\alpha = \arccos\left(1 - \frac{A_1 B_1^2}{2R_2^2}\right) \tag{11}$$

We notice that in order to find out the angle α we must find the values of the segment A_1B_1 and the radius R_2 .

We get the A_1B_1 length considering the fact that the points A_1 and B_1 have known coordinates,

$$A_1 B_1 = \sqrt{h_{cone}^2 + g_{bn}^2} \tag{12}$$

In order to determine the radius R_2 we apply Pythagoras' Theorem in the triangle $\Delta C_1 B_1 N$ and find

$$R_2 = \sqrt{\left(\frac{l_y - g_{base}}{2} - c_1\right)^2 + (x_1 - l_v)^2}$$
 (13)

Inserting the formulas (12) and (13) in the relation (11) we get the formula of the quantity a

$$\alpha = \arccos\left(1 - \frac{h_{cone}^2 + g_{bn}^2}{2\left[\left(\frac{l_y - g_{base}}{2} - c_1\right)^2 + (x_1 - l_v)^2\right]}\right)$$
(14)

In order to find the φ angle we apply generalized Pythagorean Theorem in the triangle $\Delta Q_1 C_1 Q_2$ and obtain

$$\varphi = \arccos\left(1 - \frac{d_{ns}^2}{2R_2^2}\right) \tag{15}$$

To determine the θ angle we apply the generalized Pythagorean Theorem in the triangle $\Delta Q_1 C_1 A_1$ and achieve

$$Q_1 A_1^2 = Q_1 C_1^2 + C_1 A_1^2 - 2Q_1 C_1 \cdot C_1 A_1 \cdot \cos \theta$$
 (16)
From the definition of the distance between two points we find

$$Q_1 A_1^2 = (x_1 - x_{A_1})^2 - (y_{Q_1} - y_{A_1})^2$$
(17)

Therefore, considering the formulas (16) and (17) and the fact that $\theta < \pi$ we obtain that the cosine function is bijective and its inverse arccos is uniquely determined. This means that the θ angle is uniquely determined and has the formula

$$\theta = \arccos \frac{Q_1 C_1^2 + R_2^2 - Q_1 A_1^2}{2Q_1 C_1 \cdot R_2} \tag{18}$$

We must notice that θ can be calculated only if we find the Cartesian coordinates of the point Q_1 .

The nanosphere with the center $Q_1(x_{Q_1}, y_{Q_1})$ is tangent to the top of the cone and to the wall of cone and hence we have

$$x_{Q_1} = h_{cone} + l_v - d_{ns}/2 (19)$$

$$C_1 Q_1 = R_2 + d_{ns}/2 (20)$$

From the definition of the distance between two points we find

$$C_1 Q_1^2 = (x_1 - x_{Q_1})^2 + (c_1 - y_{Q_1})^2$$
(21)

Hence, from the formulas (19), (20) and (21) we obtain the y-coordinate of the point Q_I

$$y_{Q_1} = c_1 + \sqrt{(R_2 + d_{ns}/2)^2 - (x_1 - h_{cone} - l_v + d_{ns}/2)^2}$$
 (22)

The number of the nanospheres from the inside cone walls can be find from the relations (10), (13), (14), (15), (18), (19) and (20).

4. The conditions for a charged particle from the initial plasma to be inside a nanosphere

A charged particle has an infinitesimal dimension, so we can associate an $M(x_M, v_M)$ mathematical point with it (Figure 1). The cone is a fixed target and because the nanospheres are tangent to the cone, it means that they have a fixed position.

Also, in the case when the M point doesn't belong to the area of a nanosphere from the cone walls, we must search which is the nanosphere closest to the M point. Therefore, we need to find the indices of the centers of two consecutive nanospheres, the i^{th} and $(i+1)^{th}$ nanospheres closest to the M point. Therefore, the M point will be inside an angle $Q_i\widehat{C_1Q_{i+1}}$. We must find the index i < n. It is straightforward to obtain the i index as the ratio $m(\widehat{MC_1}A_1)/\varphi$ (Figure 2(a)).

We must find the coordinates of the centers of the tangent nanospheres at the cone walls and at the top of the cone. In order to determine if the M point is inside of a nanosphere, we must obtain the distance from M to Q_i , and by using this value, the distance from M to the O_{i+1} point. Thus, we achieve the coordinates of the centers Q_i by means of a recurrence formula.

For a better understanding of how to obtain the coordinates of the Q_i centers we draw a scheme of the positions of the points C_I , A_I , Q_I and Q_i in Figure 4.

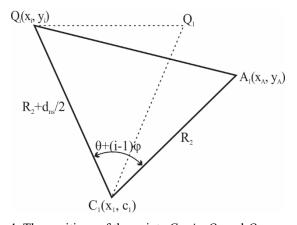


Fig. 4. The positions of the points C_l , A_l , Q_l and Q_i .

For the achievement of the coordinates of the nanosphere centers on the cone walls we apply the generalized Pythagorean Theorem in triangle $\Delta A_1 C_1 Q_i$. We get

$$(x_A^2 - x_{C_1}^2) + (y_A^2 - y_{C_1}^2) - 2(x_{A_1} - x_{C_1})x_i - 2(y_{A_1} - y_{C_1})y_i = R_{i\varphi}$$
 (23)

where $R_{i,0} \stackrel{\text{def}}{=} R_2^2 - 2R_2(R_2 + d)cos(\theta + (i - 1)\varphi)$.

We do the same in the triangle $\Delta C_1 Q_1 Q_i$ and we get

$$2(x_1 - x_{Q_1})x_i + 2(y_{C_1} - y_{Q_1})y_i - (x_1^2 - x_{Q_1}^2) - (y_{C_1}^2 - y_{Q_1}^2) = R_{i\varphi}^1$$
 where $R_{i\varphi}^1 \stackrel{\text{def}}{=} (R_2 + d)^2 - 2(R_2 + d)^2 cos((i - 1)\varphi).$ (24)

Taking into account the relations (23) and (24) we obtain a system of two equations with two variables, x_i and y_i :

$$\begin{cases}
2(x_1 - x_A)x_i + 2(y_{C_1} - y_A)y_i = R_{i\varphi} - (x_A^2 + y_A^2 - x_1^2 - y_{C_1}^2) \\
2(x_1 - x_{Q_1})x_i + 2(y_{C_1} - y_{Q_1})y_i = R_{i\varphi}^1 + (x_1^2 + y_{C_1}^2 - x_{Q_1}^2 - y_{Q_1}^2)
\end{cases}$$
We must notice that $2s \cdot y_i = R_{i\varphi}^2$ and $-2sx_i = R_{i\varphi}^3$, where
$$s = (y_{C_1} - y_{A_1})(x_1 - x_{Q_1}) - (y_{C_1} - y_{Q_1})(x_1 - x_{A_1}) \tag{25}$$

$$s = (y_{C_{1}} - y_{A_{1}})(x_{1} - x_{Q_{1}}) - (y_{C_{1}} - y_{Q_{1}})(x_{1} - x_{A_{1}})$$

$$R_{i\varphi}^{2} = R_{i\varphi} - (x_{A_{1}}^{2} + y_{A_{1}}^{2} - x_{1}^{2} - y_{C_{1}}^{2})(x_{1} - x_{Q_{1}})$$

$$- (R_{i\varphi}^{1} + x_{1}^{2} + y_{C_{1}}^{2} - x_{Q_{1}}^{2} - y_{Q_{1}}^{2})(x_{1} - x_{A_{1}})$$

$$R_{i\varphi}^{3} = (R_{i\varphi} - x_{A_{1}}^{2} - y_{A_{1}}^{2} + x_{1}^{2} + y_{C_{1}}^{2})(y_{C_{1}} - y_{Q_{1}})$$

$$- (R_{i\varphi}^{1} + x_{1}^{2} + y_{C_{1}}^{2} - x_{Q_{1}}^{2} - y_{Q_{1}}^{2})(y_{C_{1}} - y_{A_{1}})$$

$$(26)$$

We can see that the quantities defined above to simplify the calculations $R_{i\varphi}$, $R_{i\varphi}^1$, $R_{i\varphi}^2$, $R_{i\varphi}^3$ and s are known, because they are defined as function of known quantities. Therefore, from the equations (24), (25) and (26) we obtain the <u>y-coordinate</u> of the center of the i^{th} nanosphere, Q_i

$$y_i = \frac{R_{i\varphi}^2}{2s} \tag{27}$$

and the x-coordinate.

$$x_i = -\frac{R_{i\varphi}^3}{s} \tag{28}$$

For the nanospheres on the top of the cone we find the coordinates of the Q'_i , i=1,m centers also by a recurrence formula. These are straightforward to determine because we know the coordinates of the center Q_I , the diameter of a nanosphere and the small base of the inside of the cone g_{neck} . Due to the fact that the nanospheres on the top of the cone are tangent to the top of the cone we deduce that their centers have the same abscissa. From the formula (19) we obtain

$$x_{Q'_{i}} = h_{cone} + l_{v} - d_{ns}/2, i = \overline{2, m}$$
 (29)

If we look at the Figure 2(b), we deduce that $y_{Q'_i} = y_{Q'_{i-1}} + d_{ns}$. By using formula (22) we get the recurrence formula for the y-coordinate of the nanosphere center Q_i

$$y_{Q_i'} = y_{Q_1} + (i-1)d_{ns} \tag{30}$$

As explained above, in order to find out which is the nanosphere on the cone wall closest to the M point, we must first find the measure of the angle $\widehat{MC_1A_1}$. For this, we apply generalized Pythagorean Theorem in the triangle $\Delta A_1 C_1 M$ (Figure 2(a)) and get

$$m(\widehat{MC_1A_1}) = \arccos \frac{MC_1^2 + R_2^2 - MA_1^2}{R_2 \cdot MC_1}$$
(31)

Because the coordinates of the points M, C_1 and A_1 are known, the segments MC_1 and MA_1 are uniquely determined.

Considering all the formulas achieved above and the fact that a cone has a symmetry axis perpendicular to the bases of the cone, we write below an algorithm for the calculation of the position of a M point.

If $x_M > h_{cone} + l_v$ or $x_M < l_v$, then the M point is outside the cone, so it is outside the nanospheres;

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If l_v \le x_M \le h_{cone} + l_v, then
  If y_M < y_{B_1} or y_M > y_{B_2}, then the M point is outside the nanospheres;
If y_M \ge y_{B_1} and y_M \le y_{B_2}, then
  If d(M, C_1) < R_2, then the M point is outside the nanospheres;
  If R_2 \leq d(M, C_1) \leq R_2 + d_{ns}, then
     If m(\not AC_1A_1) > \theta and m(\not AC_1B_1) > \alpha - \theta, then
M \in Int(\widehat{Q_{i+1}C_1Q_i}), where i = \left[\frac{m(\sqrt[4]{M}C_1A_1) - \theta}{m}\right]
      If d(M, Q_i) \le d_{ns}/2, then M \in \mathcal{D}(Q_i, d_{ns}/2);
        If d(M, Q_i) > d_{ns}/2, then
        If d(M, Q_{i+1}) > d_{ns}/2, then the M point is outside the nanospheres;
            If d(M, Q_{i+1}) \le d_{ns}/2, then M \in \mathcal{D}(Q_{i+1}, d_{ns}/2);
         If m(\sphericalangle MC_1A_1) \leq \theta, then M \in Int(\widehat{Q_1C_1A_1})
            If d(M, Q_1) \le d_{ns}/2, then M \in \mathcal{D}(Q_1, d_{ns}/2);
            If d(M, Q_1) > d_{ns}/2, then the M point is outside the nanospheres;
        If m(\not A M C_1 B_1) \leq \alpha - \theta, then M \in Int(\widehat{B_1 C_1 Q_n})
            If d(M, Q_n) \leq d_{ns}/2, then M \in \mathcal{D}(Q_n, d_{ns}/2);
            If d(M, Q_n) > d_{ns}/2, then the M point is outside the nanospheres;
      If d(M, C_1) > R_2 + d_{ns}, then
        If h_{cone} + l_v - x_M > d_{ns}, then
        If d(M, C_2) > R_2 + d_{ns}, then the M point is outside the nanospheres;
              If d(M, C_2) < R_2, then the M point is outside the nanospheres;
              If R_2 \le d(M, C_2) \le R_2 + d_{ns}, then
         If m( \blacktriangleleft MC_2A_2) > \theta and m( \blacktriangleleft MC_2B_2) > \alpha - \theta, then
               M \in Int(\widehat{Q_{i+1}C_2Q_i}), where i = \left\lceil \frac{m(\langle MC_2A_2) - \theta}{\omega} \right\rceil;
           If d(M, Q_i) \le d_{ns}/2, then M \in \mathcal{D}(Q_i, d_{ns}/2);
            If d(M, Q_i) > d_{ns}/2, then
     If d(M, Q_{i+1}) > d_{ns}/2, then the M point is outside the nanospheres;
           If d(M, Q_{i+1}) \le d_{ns}/2, then M \in \mathcal{D}(Q_{i+1}, d_{ns}/2);
     If m(\sphericalangle MC_2A_2) \leq \theta, then M \in Int(\widehat{Q_mC_2A_2})
           If d(M, Q'_m) \le d_{ns}/2, then M \in \mathcal{D}(Q'_m, d_{ns}/2);
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If d(M,Q_m')>d_{ns}/2, then the M point is outside the nanospheres; If m(\sphericalangle MC_2B_2)\leq \alpha-\theta, then M\in Int(B_2C_2Q_n) If d(M,Q_n)\leq d_{ns}/2, then M\in \mathcal{D}(Q_n,d_{ns}/2); If d(M,Q_n)>d_{ns}/2, then the M point is outside the nanospheres; If d(M,C_2)>R_2+d_{ns}, then If d(M,C_2)>R_2+d_{ns}, then If d(M,C_2)>R_2+d_{ns}, then the M point is outside the nanospheres; If d(M,C_2)< R_2, then the M point is outside the nanospheres; If d(M,C_2)< R_2, then the M point is outside the nanospheres; If d(M,C_2)< R_2, then d(M,C_2)< R_2, then If d(M,C_2)< R_2, then d(M,C_2), then d(M,C_2)
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We named $\mathcal{D}(Q_i, d_{ns}/2)$ the disk with the center Q_i and the radius $d_{ns}/2$ which is the section in the x-y plan of the i^{th} nanosphere.

This algorithm can be used in a PIC code for the density profile of an initial plasma created at the interaction of an ultra-high intensity laser pulse with a nanostructured cone.

5. Conclusions

We described mathematically the density profile of the initial plasma created at the interaction of an ultra-high intensity laser pulse with a new nanostructured flat-top cone target. The flat-top cone is coated inside with nanospheres with the same diameter. We found the coordinates of the centers of the nanospheres which are on the top and walls of a nanostructured cone target. The formula for the number of the nanospheres was determined. We obtained the necessary and sufficient conditions for a charged particle to be inside of a nanosphere.

This profile density is dedicated to be used in PIC codes.

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