Program Documentation

Dynamics of charged micro/nano dust and debris

Analytical Model and Simulation of the trajectories of debris around the earth and dust emitted from a comet

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Resume

This document outlines the development of a test particle model to simulate the dynamics of charged micrometric objects in plasma environments, specifically focusing on cometary (dust grains) and geocentric (space debris) scenarios. The goal is to solve the equation of motion for such objects. For micron-sized objects, the Lorentz force could become much more significant, therefore playing an important role on the trajectories of these bodies. Hence, the first objective is to establish the charging currents using the thick sheath approximation, in order to predict the charge evolution over time. Initially, we detail the various charging currents to determine how charges are accumulated and vary on these micron-sized bodies. Following this, we catalog the forces involved in the dynamics of such particles. Finally, the document discusses the methods of integration and algorithms used to solve numerically the equation of motion. The ultimate goal is to provide accurate simulations that yield outputs of positions and velocities of the particles, enabling us to predict and analyze their trajectories in space environments effectively. Additionally, this document provides insights into the progression from model establishment to implementation, discusses initial analyses and interpretations of the outputs, and defines the code's limitations. Finally, suggestions for further work to build upon this foundation are presented.

Contents

1 Introduction **1**

2 Physical Model **2**
- 2.1 Charging mechanisms and physical approximations . . . 2
  - 2.1.1 Thick Sheath Approximation . . . 2
  - 2.1.2 Analysis of Plasma Sheath Theories . . . 2
- 2.2 Currents collected at a spherical body . . . 2
  - 2.2.1 Electronic currents . . . 3
  - 2.2.2 Ionic currents . . . 3
  - 2.2.3 Photo-emission currents . . . 4
  - 2.2.4 Secondary electronic current emission . . . 4
  - 2.2.5 Thermionic current emission . . . 5
  - 2.2.6 Backscattered electronic emission . . . 5
- 2.3 Grain charge expression . . . 5
- 2.4 Dynamics of a grain in different environments . . . 6
  - 2.4.1 Equation of motion for charged dust in the cometary's environment . . . 6
  - 2.4.2 Equation of motion for charged debris in the Earth's environment . . . 9

3 Algorithm and integration methods **11**
- 3.1 Dichotomy method to estimate the equilibrium surface potential . . . 11
- 3.2 Runge-Kutta method to integrate the current balance equation . . . 12
- 3.3 Boris algorithm for the motion of charged particles emerged in fields . . . 12
- 3.4 Sketch of the Python script . . . 14

4 Others Programs **14**
- 4.1 Representation of dynamics . . . 14
- 4.2 Forces validation . . . 15
- 4.3 Validation and verification of the charge update . . . 17
  - 4.3.1 Order of Convergence Study . . . 17
  - 4.3.2 Methodology for Verifying Half and Full Implementations . . . 17
- 4.4 Evolution of the charging currents . . . 18
- 4.5 Balance of the forces . . . 20

5 Perspectives **20**
- 5.1 Limits of the model . . . 20
- 5.2 Suggestions to continue this work . . . 21

1 Introduction

This study aims to develop a comprehensive model to simulate the dynamics of charged micro/nano dust and debris in various plasma environments, specifically focusing on cometary and geocentric scenarios. The key challenge is to integrate simultaneously two critical equations: the non-quasi-static equilibrium of charge currents and the equation of motion considering all relevant forces.

Accurate numerical methods are crucial for these simulations. We utilize the Runge-Kutta (RK4) method to solve the charge equilibrium equation and the Boris Push algorithm to solve the equation of motion. The RK4 method helps determine how the charge on a micro-sized object evolves over time in a magnetized plasma, while the Boris Push algorithm computes the object's trajectory under the influence of multiple forces.

The physical model involves detailed charging mechanisms and various physical approximations. We adopt the thick sheath approximation, where the Debye length of the plasma is significantly larger than the object's characteristic length. This leads to a dominant role of extended electrostatic forces. The collected currents, including electronic, ionic, photo-emission, secondary electronic emission, thermionic emission, and backscattered electronic currents, are computed using established theories like the Orbit Motion Limit (OML) theory.

The equation of motion for charged dust in cometary and terrestrial environments considers forces such as Lorentz force, solar radiation pressure, solar gravity, gas drag, and nucleus gravity. In the cometary environment, the dynamics are influenced by different regions around the comet, such as the coupled coma, transitional coma, and the trail. For the terrestrial environment, we consider geocentric equatorial inertial coordinates and additional forces like the oblateness of the planet and atmospheric drag.

To solve the complex equations, we implement several numerical methods. The dichotomy method estimates the equilibrium surface potential by balancing the currents. The RK4 method integrates the current balance equation to determine the grain's charge over time. The Boris Push algorithm computes the positions and velocities of charged particles immersed in electromagnetic fields.

To ensure the accuracy of our model, we validate the implementation of each force and the charge update mechanism. For the charge update, we specifically developed a methodology to compare the half and full implementations of the Boris Push algorithm against an analytical model. Although this work is still ongoing and hasn't yielded conclusive results, it forms a basis for further study.

Additional scripts were developed to visualize the 3D trajectories of dust and debris, validate the implementation of forces, compare the contributions of different forces, and analyze the evolution of charging currents over time. These programs support the main simulation by providing detailed insights into specific aspects of the particle dynamics.

While our initial results are promising, this study is only an introduction. Future work will focus on optimizing the RK4 implementation within the Boris Push framework. Potential areas of further research include addressing numerical stability issues in the Boris Push method for extremely small time steps and exploring hybrid methods to improve accuracy and stability in long-term simulations.

2 Physical Model

2.1 Charging mechanisms and physical approximations

2.1.1 Thick Sheath Approximation

In the context of plasma sheath models, the thick sheath approximation is used when the Debye length (λ_D) of the plasma is significantly larger than the characteristic length of the object (r_s), i.e., $\lambda_D \gg r_s$. This condition leads to a "thick" plasma sheath [1], where the electrostatic shielding extends far from the object's surface. The main implications of this approximation are:

- Enhanced electrostatic influence on charged particles in the plasma.
- Altered charge collection dynamics at the object's surface.

This approximation simplifies the analysis of plasma-object interactions by assuming a dominant role of extended electrostatic forces.

2.1.2 Analysis of Plasma Sheath Theories

In this analytic model, the currents collected in the thick sheath regime are computed using the Orbit Motion Limit (OML) theory. Initially introduced by Mott-Smith and Langmuir in 1926 [2], OML has become the predominant theory for dust charging. It is based on the conservation of angular momentum and energy within the plasma sheath. OML theory typically considers bodies of simple geometrical shapes, such as spherical or cylindrical. For the rest of the study, we approximate the debris and dust grains to a sphere.

While the focus of this document is on the application of OML theory, it is important to acknowledge other significant theories in the study of plasma sheaths:

- **Allen Boyd Reynolds (ABR) theory**: This theory considers radial movements of ions at the edge of the sheath, influenced by the spacecraft potential. [3]
- **Bernstein Rabinowitz Laframboise (BRL) theory**: BRL is an extension that combines elements of both OML and ABR, accounting for a variety of particle trajectories and energy states. [4]

These theories provide additional perspectives on plasma interactions, but for the purposes of this analysis, the simplified approach of OML is preferred due to its direct applicability to the debris and dust grains.

2.2 Currents collected at a spherical body

The following sections detail the expressions of the charging currents. More details can be found in the references associated.

2.2.1 Electronic currents

Reference : [5]

$$
\begin{aligned}
I_e &= -4\pi r_s^2 e n_e \sqrt{\frac{k_B T_e}{2\pi m_e}} \exp\left(-\frac{e|\phi|}{k_B T_e}\right) && \text{if } \phi < 0 \\
I_{e0} &= -4\pi r_s^2 e n_e \sqrt{\frac{k_B T_e}{2\pi m_e}} && \text{if } \phi = 0 \\
I_e &= -4\pi r_s^2 e n_e \sqrt{\frac{k_B T_e}{2\pi m_e}} \left(1 + \frac{e\phi}{k_B T_e}\right) && \text{if } \phi > 0
\end{aligned}
$$

Inputs : r_s, n_e, T_e, ϕ
Output : Electron current

- r_s is the radius of the sphere
- n_e is the plasma electrons density
- T_e is the plasma electrons temperature
- ϕ is the potential at the surface of the body
- k_B is the Boltzmann constant
- e is the elementary charge
- m_e is the mass of the electron

2.2.2 Ionic currents

Reference : [5]

$$
\begin{aligned}
I_i &= 4\pi r_s^2 e n_i \sqrt{\frac{k_B T_i}{2\pi m_i}} \exp\left(-\frac{e\phi}{k_B T_i}\right) && \text{if } \phi > 0 \\
I_{i0} &= 4\pi r_s^2 e n_i \sqrt{\frac{k_B T_i}{2\pi m_i}} && \text{if } \phi = 0 \\
I_i &= 4\pi r_s^2 e n_i \sqrt{\frac{k_B T_i}{2\pi m_i}} \left(1 - \frac{e\phi}{k_B T_i}\right) && \text{if } \phi < 0
\end{aligned}
$$

Inputs : r_s, n_i, T_i, ϕ
Output : Ion current

- r_s is the radius of the sphere
- n_i is the plasma ions density
- T_i is the plasma ion's temperature
- m_i is the mass of the ion

2.2.3 Photo-emission currents

Reference : [6]

$$I_{\text{ph}} = \pi r_s^2 e \left(\frac{y \times 10^{14} \times \gamma}{d_{\text{AU}}^2} \right) \qquad \text{if } \phi < 0$$
$$I_{\text{ph}} = \pi r_s^2 e \left(\frac{y \times 10^{14} \times \gamma}{d_{\text{AU}}^2} \right) \exp\left(\frac{-e\phi}{k_B T_{\text{ph}}} \right) \left(1 + \frac{e\phi}{k_B T_{\text{ph}}} \right) \qquad \text{if } \phi > 0$$
$$I_{\text{ph}} = \pi r_s^2 e \left(\frac{y \times 10^{14} \times \gamma}{d_{\text{AU}}^2} \right) \qquad \text{if } \phi = 0$$

Inputs : r_s**,** T_{ph}**,** γ**,** y**,** d_{AU}**,** ϕ
Output : Photoelectrons current

- T_{ph} is the plasma photoelectrons temperature.
- d_{AU} is the distance from the sun in astronomical units AU.
- y is the photoemission yield (the number of photoelectrons emitted per incident photon).
- γ is the solar photon flux.

2.2.4 Secondary electronic current emission

Reference : [6]

$$I_{\text{sec}} = 3.7 \delta_M I_{0e} \exp\left(\frac{e\phi}{k_B T_{\text{e}}} \right) F_5 \left(\frac{E_M}{4 k_B T_e} \right) \qquad \text{if } \phi < 0$$
$$I_{\text{sec}} = 3.7 \delta_M I_{0e} \left(1 + \frac{e\phi}{k_B T_{\text{s}}} \right) \exp\left(\frac{-e\phi}{k_B T_{\text{s}}} \right) F_{5,B} \left(\frac{E_M}{4 k_B T_e} \right) \qquad \text{if } \phi > 0$$
$$F_5(x) = x^2 \int_0^\infty u^5 e^{-(xu^2+u)}\, du$$
$$F_{5,B}(x) = x^2 \int_B^\infty u^5 \exp[-(xu^2+u)]\, du$$
$$B = \left(\frac{\left(\frac{e\phi}{k_B T_{\text{e}}} \right)}{\frac{E_M}{4 k_B T_e}} \right)^{1/2}$$

Inputs : I_{0e}**,** T_e**,** T_{sec}**,** δ_M**,** E_M**,** ϕ
Output : Secondary electron current

- I_{0e} is the electron current at zero potential.
- T_{s} is the secondary temperature.
- δ_M is the maximum yield. Depends on material.
- E_M is the optimum primary energy (energy at maximum yield). Depends on material.
- The functions $F_5(x)$ and $F_{5,B}(x)$ are integrals defined for the appropriate conditions.
- B is the upper limit of the integral, depending on the potential and energy of the electrons.

2.2.5 Thermionic current emission

Reference : [7]

$$I_{\text{th}} = -4\pi r_s^2 A_r T_d^2 \exp\left(-\frac{eW_f}{k_B T_d}\right)$$

Inputs : T_d**,** r_s**,** W_f
Output : Thermionic current

- T_d is the temperature at the surface of the grain/debris
- A_r is the Richardson's constant : $A_r = 1,20173 \times 10^6 Am^{-2}K^{-2}$
- W_f is the work function of the material in eV

2.2.6 Backscattered electronic emission

Reference : [8]

$$\begin{aligned} I_{\text{bs}} &= 0 && \text{if } E_{\text{bs}} < E_{\text{min}} \\ I_{\text{bs}} &= 0.3\, I_e && \text{if } E_{\text{bs}} \geq E_{\text{min}} \\ E_{\text{bs}} &= (0.45 + 2 \times 10^{-3} \cdot z) \cdot (k_B T_e + (e \cdot \phi)) \end{aligned}$$

Inputs : I_e**,** T_e**,** z**,** ϕ
Output : Backscattered electronic current

- I_e is the electronic current
- E_{bs} is the resulting energy of the backscattered electrons.
- E_{min} = 100 eV is the energy distribution of the backscattered electrons.
- z is the atomic number of the target.

2.3 Grain charge expression

The grain charge $Q(t)$ is given by the following expression:

$$\frac{dQ}{dt} = \sum I \approx I_{ph} + I_e + I_i + I_s + I_{th} + I_{BS}, \tag{1}$$

from [6] With $Q = \Phi C$ where C is the capacitance : $C = 4\pi\varepsilon_0 r_s$

2.4 Dynamics of a grain in different environments

2.4.1 Equation of motion for charged dust in the cometary's environment

Referential considered The cometocentric reference frame is defined as :

- **Axis X:** It is aligned with the direction of the sun at a given moment. This means that the X-axis points from the center of the comet towards the sun.
- **Axis Y:** It is perpendicular to the X-axis in the plane formed by the comet's orbit.
- **Axis Z:** It is taken to be perpendicular to the plane formed by the X and Y axes. This axis is aligned with the orbital angular momentum of the comet, meaning it points along the direction of the orbit's rotational axis.

In this case we have to considerate 7 forces : Lorentz force, Solar radiation pressure, Solar gravity, Gas drag, comet gravity, radial tidal force and finally Poynting-Robertson drag

In a cometary environment, we have 3 zones defined by the nucleus radius R_N and the Hill sphere, sphere of gravitational influence $R_{Hill} = d\left(\frac{1}{3}\frac{M_{\text{comet}}}{M_\odot}\right)^{\frac{1}{3}}$ (d is the heliocentric distance of the comet ; M_{comet} is the mass of the comet ; $M_\odot$ is the mass of the Sun):

- **The coupled coma :** $(0-10R_N)$ The dynamic of a grain in this region is dominate by Gas drag (because $D_{inter-grain} << \lambda_D$), nucleus gravity and Electromagnetic forces.
- **Transitional coma :** $(10R_N - 1R_{Hill})$ The dynamic here is dominate by Solar radiation, Electromagnetic forces and also nucleus gavity.
- **Trail :** $(1R_{Hill} - \infty)$ Finally, in this region the dominant force is the solar force.

Reference : [9]

For exemple at $r > 20km$ and $d >> 1$, we can consider only electromagnetic forces and solar radiation pression from [10].

For a general formulation ,the resulting equation of motion considering all forces is given by :

$$\frac{md\vec{v}}{dt} = \vec{F}_{\text{Electromagnetic}} + \vec{F}_{\text{Radiation}} + \vec{F}_{\text{Gas drag}} + \vec{F}_{\text{Comet gravity}} + \vec{F}_{\text{Tidal gravity}} + \vec{F}_{\text{Solar gravity}} + \vec{F}_{\text{Poynting-Robertson drag}} \tag{2}$$

Electromagnetic force

$$\vec{F}_{\text{Lorentz}} = Q(t)\left(\vec{E} + \frac{\vec{v}_{\text{drift}} \times \vec{B}}{c}\right) \tag{3}$$

$$\vec{E} = -\frac{\vec{v_p} \times \vec{B}}{c}. \tag{4}$$

Inputs : $Q(t)$, $\vec{E}$, $\vec{v}_{\textbf{drift}}$, $\vec{B}$, $\vec{v_p}$
Output : $\vec{F_L}$

- $\vec{v}_{\text{drift}}$ is the drift velocity of particle.
- $\vec{v_p}$ is the plasma velocity.
- $Q(t)$ is the charge of the grain.
- c is the speed of light.
- $\vec{E}$ and $\vec{B}$ are the electric and magnetic fields.

Solar radiation pressure force
Reference : [10]

$$\vec{F_r} = \frac{Q_{pr} L_{\odot} r_s^2}{c} \left(\frac{\vec{r_{\odot}} - \vec{r_{\text{grain}}}}{|\vec{r_{\odot}} - \vec{r_{\text{grain}}}|^3} \right) \tag{5}$$

Inputs : Q_{pr}**,** d**,** $L_{\odot}$**,** r_s
Output : $\vec{F_r}$

- Q_{pr} : scattering efficiency for radiation pressure.
- $L_{\odot}$: luminosity of the Sun.
- $\vec{r_{\odot}}$ is the position vector of the sun
- $\vec{r_{\text{grain}}}$ is the position of the grain

Gravity forces
Reference : [9]

Solar gravity expression :

$$\vec{F}_{\text{solar}} = GM_{\odot} m \left(\frac{\vec{r_{\odot}} - \vec{r_{\text{grain}}}}{|\vec{r_{\odot}} - \vec{r_{\text{grain}}}|^3} \right) - \left(\frac{\vec{r_{\odot}}}{|\vec{r_{\odot}}|^3} \right) \tag{6}$$

Comet gravity expression :

$$\vec{F}_{\text{comet}} = GM_{\text{comet}} m \left(\frac{\vec{r_{\odot}}}{|\vec{r_{\odot}}|^3} \right) \tag{7}$$

Radial Tidal force :

$$\vec{F}_{\text{Tidal}} = -\left(\frac{2GM_{\odot}}{d^3} \right) m r_c \left(\frac{\frac{\vec{r_{\text{grain}}}}{|\vec{r_{\text{grain}}}|}}{|\vec{r_{\odot}} - \vec{r_{\text{grain}}}|^3} \right) \tag{8}$$

Inputs : m**,** d**,**$M_{\textbf{comet}}$**,** r_c
Output : $\vec{F}_{\textbf{Comet gravity}}$**,** $\vec{F}_{\textbf{Solar gravity}}$, $\vec{F}_{\text{Tidal force}}$

- m is the mass of the grain.
- M_{comet} is the mass of the comet.

- $M_\odot$ is the mass of the sun.
- r_c is the distance of the grain from the comet.
- d is the distance from the sun.
- $\vec{r_\odot}$ is the position vector of the sun
- $\vec{r_{\text{grain}}}$ is the position of the grain
- $G = 6,668 \times 10^{-11} kg^{-1} s^{-2} m^3$ is the gravitational constant.

Gas drag force

Reference : [9]

The drag force, $\vec{F}_D$, on a spherical particle is given by:

$$\vec{F}_D = -\frac{1}{2} C_D m_g n_g \pi r_s^2 |\vec{v}_{rel}| \vec{v}_{rel}, \tag{9}$$

The drag coefficient C_D is defined, for an equilibrium gas flow and a mean free path of the molecules much larger than the dust size, by:

$$C_D = \frac{2\xi^2 + 1}{\sqrt{\pi \xi^3}} e^{-\xi^2} + \frac{4\xi^4 + 4\xi^2 - 1}{2\xi^4} \operatorname{erf}(\xi) + \frac{2(1-\varepsilon)\sqrt{\frac{\pi T_d}{T_g}}}{3\xi}, \tag{10}$$

where :

$$\xi = \frac{|\vec{v}_g - \vec{v}_d|}{\sqrt{\frac{2k_b T_g}{m_g}}}, \tag{11}$$

- m_g is the mass of a gas molecule.
- n_g is the number density.
- $\vec{v}_{rel}$ is the grain velocity relative to the gas.
- C_D is the drag coefficient.
- T_g is the gas temperature.
- T_d is the dust temperature.
- ε is the fraction of specular reflection.
- ξ is the molecular speed ration.
- $\vec{v_g}$ is the gas speed in coma
- $\vec{v_d}$ is the dust speed

Inputs : $T_g, T_d, m_g, n_g, r_s, \vec{v}_{Dust}, \vec{v}_{drift}, \vec{v}_g, \vec{v}_d$
Output : $\vec{F}_{\mathbf{Drag}}$

Poynting-Robertson drag
Reference : [10] [9]

$$\vec{F}_{PR} = \frac{{r_s}^2 L_{\odot}}{4c^2}\sqrt{GM_{\odot}}\left(\frac{\vec{v_{\text{grain}}}}{|\vec{v_{\text{grain}}}|}\frac{1}{\sqrt{\left\|\vec{r_{\odot}} - \vec{r_{\text{grain}}}\right\|^5}}\right) \tag{12}$$

Inputs : $d, L_{\odot}, r_s$
Output : $\vec{F}_{\textbf{Poynting-Robertson drag}}$

- $L_{\odot}$ is the luminosity of the Sun, $L_{\odot} = 3,826 \times 10^{26}\ Js^{-1}$.
- $\vec{v}$ is the velocity of the grain/debris.
- d is the distance from the sun.

2.4.2 Equation of motion for charged debris in the Earth's environment

Reference : [11] [12]
Geocentric equatorial inertial coordinate system (GEI) is chosen to follow the position of the debris.

- **Axis X:** Points from the Earth toward the position of the Sun at the vernal equinox.
- **Axis Z:** Parallel to the rotation axis of the Earth
- **Axis Y:** Completes the right-hand coordinate system

Equation of motion :

$$\begin{aligned} m\frac{d^2\mathbf{r}}{dt^2} = &-\frac{GmM_E}{r^2}\left[1 - \frac{3}{2}J_2\left(\frac{R_E}{r}\right)^2(3\cos^2\theta - 1)\right]\mathbf{e}_r \\ &- \frac{3GmM_E}{r^2}J_2\left(\frac{R_M}{r}\right)^2\cos\theta\sin\theta\mathbf{e}_\theta \\ &- \frac{Q_{pr}r_s^2L_{\odot}}{cd^2}\frac{(\mathbf{R}-\mathbf{r})}{|\mathbf{R}-\mathbf{r}|^3} \\ &+ GmM_{\odot}\left(\frac{(\mathbf{R}-\mathbf{r})}{|\mathbf{R}-\mathbf{r}|^3} - \frac{\mathbf{R}}{R^3}\right) + Q(t)\left(\mathbf{E} + \frac{d\mathbf{r}}{dt}\times\frac{\mathbf{B}}{c}\right) \end{aligned} \tag{13}$$

The two first terms represent the gravitational force of the Earth. The third term represent the radiation pressure force. The fourth term is the solar gravity. Fifth term is the Lorentz force.

- m is the mass of the body
- r is the distance from the Earth

- G : gravitational constant, $G = 6,668 \times 10^{-11} kg^{-1} s^{-2} m^3$
- M_E : mass of the planet, $M_E = 5,9742 \times 10^{27} g$
- R_E : radius of Earth, $R_E = 6378 km$
- R_M : radius of the moon, $R_M = 1737,4 km$
- J_2 : oblateness of the planet, $J_2 = 1,082 \times 10^{-3}$
- $L_\odot$: luminosity of the Sun, $L_\odot = 3,826 \times 10^{26}\ Js^{-1}$
- d is the distance from the sun
- Q_{pr} : lightscattering efficiency, depends on the size, composition and surface properties of the body
- $M_\odot$: solar mass, $M_\odot = 1,99 \times 10^{30} kg$
- **R** is the position vector of the sun
- **E** and **B** are the local electric and magnetic fields

Let us convert the two first terms in equation (14) into Cartesian coordinates.
Using :

$$
\begin{aligned}
r &= \sqrt{x^2 + y^2 + z^2} \\
\theta &= \arccos\left(\frac{z}{r}\right) \\
\phi &= \arctan 2(y, x)
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{e}_r &= \sin\theta\cos\phi\ \mathbf{e_x} + \sin\theta\sin\phi\ \mathbf{e_y} + \cos\theta\ \mathbf{e_z} \\
\mathbf{e}_\theta &= \cos\theta\cos\phi\ \mathbf{e_x} + \cos\theta\sin\phi\ \mathbf{e_y} - \sin\theta\ \mathbf{e_z}
\end{aligned}
$$

One can write the term of the gravitational force of the Earth as :

$$
\begin{aligned}
m\frac{d^2\mathbf{r}}{dt^2} = &-\frac{GmM_E}{r^3}\left[1 - \frac{3}{2}J_2\left(\frac{R_E}{r}\right)^2(3\frac{z^2}{r^2} - 1)\right](x\vec{e}_x + y\vec{e}_y + z\vec{e}_z) \\
&- \frac{3GmM_E}{r^5}J_2\left(\frac{R_M}{r}\right)^2\left(xz^2\vec{e}_x + yz^2\vec{e}_y - (x^2+y^2)\vec{e}_z\right)
\end{aligned}
\tag{14}
$$

Where we take the vectors $\vec{e}_x$, $\vec{e}_y$, $\vec{e}_z$ in the same directions as the GEI coordinate system.

Note that the reference used does not include the interparticle Coulomb interactions as well as the atmospheric drag forces.

[Horanyi et al., 1989] [8] assumes the interparticle distances to be larger than the Debye length, therefore neglecting the inter-debris Coulomb interactions.

[Smriti Paul and Frueh Carolin] [12] gives the expression of the atmospheric drag force :

$$\mathbf{F_{drag}} = -\frac{1}{2} C m_g n_g \pi r_s^2 |\vec{v}_{rel}| \vec{v}_{rel} \tag{15}$$

where :

- C is the drag coefficient.
- n_g is the atmospheric number density.
- m_g is the mass of a gas molecule.
- $\vec{v}_{rel}$ is the velocity of the body relative to the gas.

The expression of the Poyting-Robertson drag can be written as the same as the one written in section 2.4.1.

3 Algorithm and integration methods

3.1 Dichotomy method to estimate the equilibrium surface potential

Reference : [13]
We use the Dichotomy (or Bisection) method to estimate the equilibrium surface potential of the body. In other words this method is used to solve numerically equation (1) when the sum of the currents is zero (therefore when the currents are balanced). The method is valid for a continuous function f on the interval $[a, b]$ which takes values of different signs at the end points of the interval and which has a single root within [a,b]. A simplified version of the algorithm is given below.

1. Let f(x) = 0 be the equation to solve for the real variable x.
2. Check if f(a) $\times$ f(b) $<$ 0. In order to have an existing solution, the function must take values at different signs at the end points.
3. Calculate the mid point c of the interval, $c = \frac{a+b}{2}$. If f(c) = 0, then c is taken as the solution.
4. Examine the sign of f(c) and replace one of the end points by (c,f(c)) so that the new interval contains the root within it.
5. Iterate until finding f(c) = 0 or when the convergence is satisfying.

In our case, a and b are chosen large enough to contain the existing root. The function f(x) is the sum of the currents and x stands for the surface potential.

3.2 Runge-Kutta method to integrate the current balance equation

Reference : [14] [15]
Equation (1) in section 2.3 suggests that the grain's charge depend on the collected currents by the spherical object. Yet, the currents themselves depend on the surface potential of the body, therefore the grain's charge. To integrate the current balance equation (1), we use the fourth order Runge-Kutta method. RK4 is a numerical method for solving ordinary differential equations, commonly used for its satisfying precision (since the total accumulated error is on the order of $O(h^4)$) and its relatively simple implementation. A simplified version of the RK4 algorithm is given below.

Let an initial value problem be specified as follows :

$$\frac{dy}{dt} = f(t,y) \ , \ y(t_0) = y_0 \tag{16}$$

y is a function of time which we would like to approximate. $\frac{dy}{dt}$ is the rate at which y changes and is a function of t and y itself. The initial values are given by (t_0, y_0). The goal is to calculate four intermediate slopes k_1, k_2, k_3 and k_4; which are weighted averages of slopes at different points within the interval; to estimate the next value of y.

For a step-size h > 0, the slopes expressions are written as:

$$\begin{aligned}
k_1 &= f(t_n, y_n) \\
k_2 &= f(t_n + \frac{h}{2}, y_n + h\frac{k_1}{2}) \\
k_3 &= f(t_n + \frac{h}{2}, y_n + h\frac{k_2}{2}) \\
k_4 &= f(t_n + h, y_n + hk_3)
\end{aligned}$$

Finally :

$$\begin{aligned}
y_{n+1} &= y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) \\
t_{n+1} &= t_n + h
\end{aligned}$$

In our case, y is the body's surface potential and $f(t,y)$ is the sum of the current. Usually starting from an uncharged surface (y_0), we integrate equation (1) to follow the body potential (therefore the charge) history until it reaches equilibrium.

An example of the evolution of the currents and the history of the charge in time, for dust grains, can be found in [6] and [8].

3.3 Boris algorithm for the motion of charged particles emerged in fields

Reference : [16] [17]

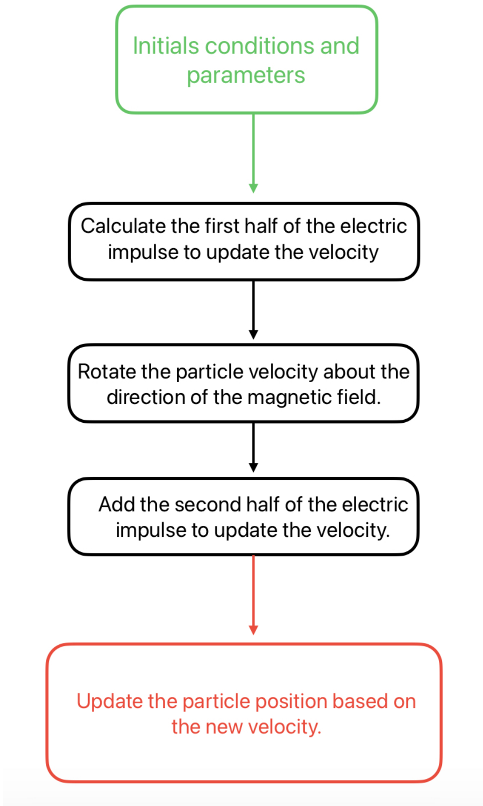


Figure 1: Flow cart of Boris Push algorithm

The Boris algorithm is used to compute the positions and velocities of particles in one or several fields. The first step involves initializing arrays to consider fields and variables. In a simple case involving the electromagnetic force, we have variables such as: $\vec{x}_i$, $\vec{v}_i$, $\vec{B}$, $\vec{E}$, q, m, and dt (time step). The method is divided into three main parts:

Adding half of the impulse from the electric field

$$\text{First half-step : } \vec{v_{\text{minus}}} = \vec{v}_i + \left(0.5 \cdot dt \cdot \frac{q}{m}\right) \cdot \vec{E}$$

Rotate the particle velocity about the direction of the magnetic field

$$\vec{t} = \vec{B} \cdot \left(0.5 \cdot dt \cdot \frac{q}{m}\right) \qquad \text{Rotation calculus}$$
$$\vec{s} = \frac{2 \cdot \vec{t}}{1 + ||\vec{t}||^2}$$

$$\vec{v_{\text{prime}}} = \vec{v_{\text{minus}}} + \vec{v_{\text{minus}}} \cdot \vec{t}$$
$$\vec{v_{\text{plus}}} = \vec{v_{\text{minus}}} + \vec{v_{\text{prime}}} \cdot \vec{s} \qquad \text{To finalize the rotation}$$

Add the second half of the impulse from the electric field

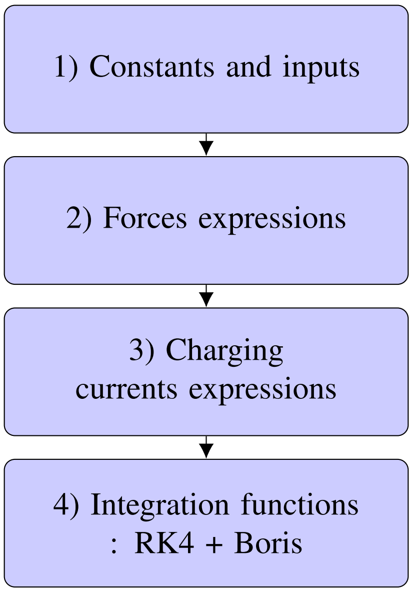
Finally, in this step we choose - with the ”inplace” function (True/False) - if we put new positions and velocity instead of the previous one in array.

$$\text{Second half-step : } \vec{v} = \vec{v_{\text{plus}}} + \left(0.5 \cdot dt \cdot \frac{q}{m}\right) \cdot \vec{E}$$

This section concludes the update of velocity. Following this, the position x would typically be updated based on the new velocity.

$$\text{Final } x \text{ position : } \vec{x} = \vec{x_i} + \vec{v} \cdot dt$$

3.4 Sketch of the Python script



This sketch represents the whole simulation. In reality, the script is decomposed in different python files such as : the constants; the inputs and the source program with all the necessary forces, charging currents expressions and the RK4 and Boris pusher algorithm. These 3 files constitute the main part of the simulation, since we can use the Boris to calculate the positions and velocities in many scenarios and for different purposes.

4 Others Programs

In addition to the three main files, there are 4 other files to : plot the trajectories in 3D; validate the implementation of the forces and the charge; compare the forces for different sizes and masses of grain and plot the evolution of the charging currents over time.

4.1 Representation of dynamics

This Python program is designed to simulate and visualize the 3D trajectories of dust/debris around the comet/Earth. The program imports the source code that calculates the positions and velocities (outputs of the Boris). Depending on the environment, the simulation either tracks particles ejected from a comet, forming its tail, or particles interacting with the Earth's electromagnetic field. To do so, the program asks the user at the beginning for the environment wanted : comet/debris.

For the comet scenario, particles are emitted from the comet's surface, with their positions and velocities updated at each time step. The program simulates how these particles move under the influence of the comet's velocity and surrounding electromagnetic fields. It checks for collisions with the comet, stopping the particles if they collide. The resulting trajectories are plotted in 3D using Plotly, with a dark theme to represent the space environment.

In the Earth's environment, the simulation follows a similar process but focuses on debris around the Earth. The trajectories are visualized with a sphere representing the Earth at the origin. Potential collisions with Earth are monitored, meaning that the debris are stopped once they collide with the blue sphere. Here, we also use Plotly to visualize the positions over time. The time of simulation is defined as 1 orbital period (calculated in the inputs file).

All the inputs that will affect the trajectories can be changed in the inputs file. In this file, you can also choose the number of grains or debris that you want to use in the simulation.

Here's an example of a figure for the comet :

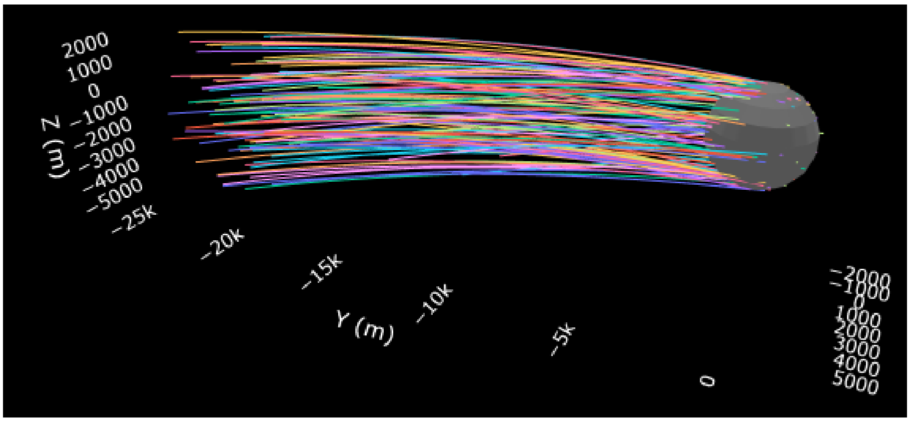


Figure 2: Representation 3D of dust grains trajectories around acomet

To visualize the trajectories : choose your inputs in the inputs file, run the trajectories file and specify the environment. A page containing the figure will open in your browser.

4.2 Forces validation

In this section, the idea is to validate the implementation of each force in the Boris. When validating a specific force, we eliminate all the other forces manipulating constants or inputs. Then we integrate the force expression to calculate a basic expression of the position and velocities over time. Finally we plot the norm of the velocity of the body over time, for both the analytical and the Boris methods. We also plot the relative error between the two curves, using :

$$\Delta = \frac{v_{numerical} - v_{analytical}}{\frac{1}{2}(v_{numerical} + v_{analytical})} \tag{17}$$

Example : if one wish to verify the implementation of the force of the solar gravity. Enter the correct inputs in the inputs file. Run the validation file : specify the environment,

the type of validation wanted (forces or the charge) and finally enter which force you would like to analyze. The program is build to automatically send the plots for the different forces. The figure below shows an example of what can be obtained when running the program.

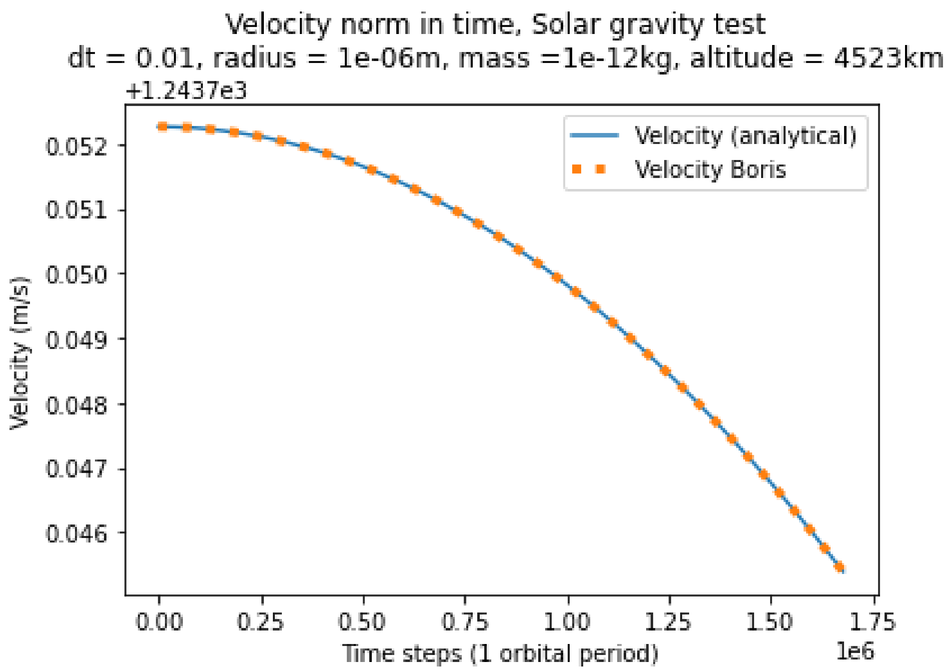


Figure 3: Velocity norm in time : Analytic / Boris implementation

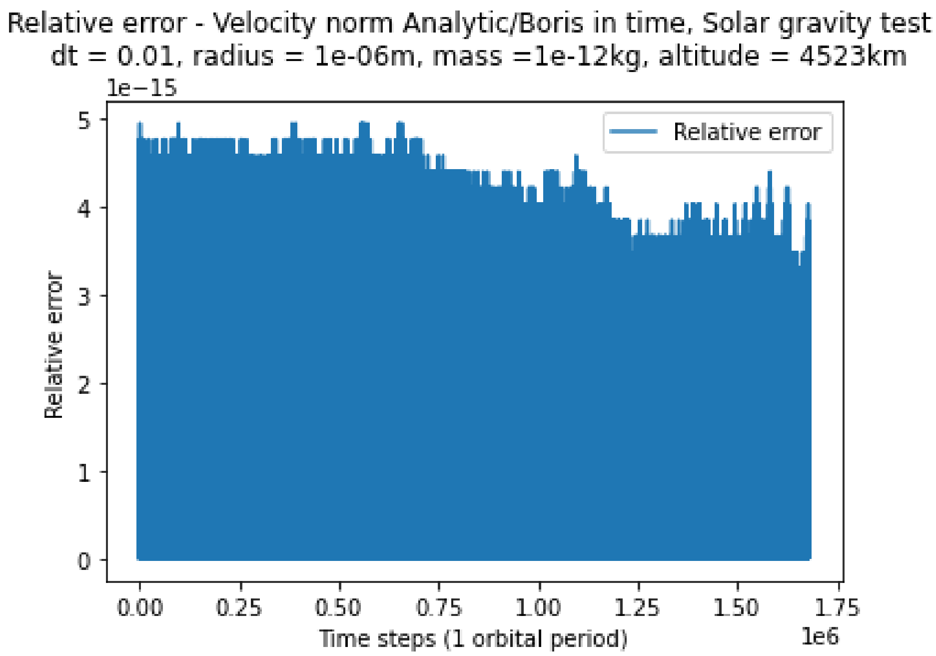


Figure 4: Relative error between analytic and boris implementation, see figure 3

This two plots can be obtained for both debris and dust environments and for each force.

Beware that, in this section, we don't really analyze the physical results but just the comparison between the analytical and numerical results.

4.3 Validation and verification of the charge update

4.3.1 Order of Convergence Study

In our study, we aimed to validate the order of convergence for both the Boris Push and the Runge-Kutta (RK4) methods. The primary focus was on confirming the theoretical convergence rates:

- For the Boris Push method, the velocity convergence follows a first-order trend while the position convergence adheres to a second-order trend.
- For the Runge-Kutta method (RK4), the convergence is expected to follow a fourth-order trend.

These theoretical expectations were confirmed through our numerical simulations, demonstrating the accuracy and stability of both the Boris Push and RK4 algorithms in the context of charged particle motion.

4.3.2 Methodology for Verifying Half and Full Implementations

To evaluate the effectiveness of the half and full implementations of the Boris Push algorithm, we developed a methodology that involves an analytical model to simulate charge evolution and the magnetic field gradient. The steps of this methodology are as follows:

- **Analytical Model Setup**: Define the magnetic field as a function of position and its gradient. Establish a charge evolution model based on the position of the particle.
- **Simulation of Half and Full Implementations**: Implement the Boris Push algorithm with both half and full charge updates. Run the simulations to update position, velocity, and charge over a series of time steps.
- **Comparison with Analytical Model**: Use the analytical model to derive the drift velocity due to the magnetic field gradient. Compare the velocities obtained from the half and full Boris Push implementations with the analytical drift velocity.
- **Error Analysis**: Analyze the errors between these methods to assess the accuracy and convergence.

Despite following this methodology, our initial attempts did not yield conclusive results. The comparison of the velocities and charges obtained from the half and full implementations with the analytical model showed discrepancies. These discrepancies suggest areas for further refinement and optimization.

This validation process is ongoing, and it is clear that further work is necessary to achieve definitive results. Future studies should focus on enhancing the accuracy and efficiency of these methods. By continuing to develop and refine this approach, we aim to achieve a robust and reliable simulation framework for charged particle dynamics in plasma environments.

Overall, the implementation of this comparative study underscores the importance of continuous validation and verification in numerical simulations. The results so far indicate that this is a promising but incomplete step, highlighting the need for further investigation to fully understand and optimize the integration of the RK4 method within the Boris Push framework.

4.4 Evolution of the charging currents

This program is designed to estimate the evolution of the charging currents over time. The idea is to run the RK4 algorithm to estimate the surface potential over time, therefore calculating the currents at each instant as well. The program plots the evolution of the currents as a function of the potential at the surface, also as a function of the time and finally the evolution of the potential over time. This could be useful to analyze which current is dominant when testing different configurations of plasma inputs. It could also be benefit to know how the currents react to different values of potential.

Here's an example of the results obtained by this program :

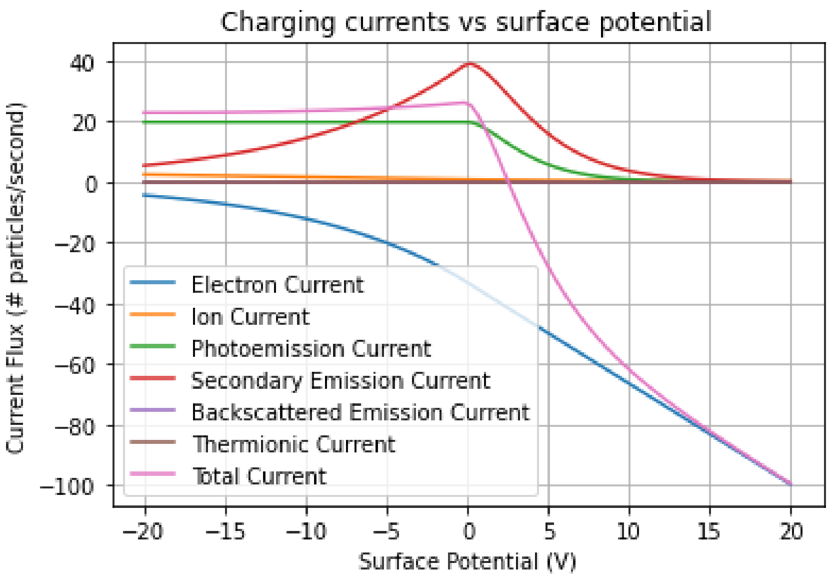


Figure 5: Evolution of the currents as a function of the potential, T_e = 10 eV, $n = 5\ cm^{-3}$

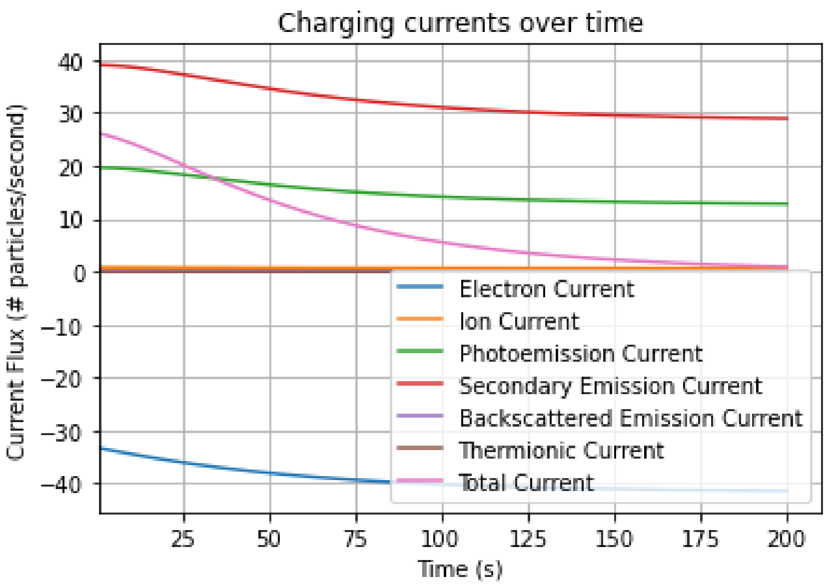


Figure 6: Evolution of the currents as a function of the potential, T_e = 10 eV, $n = 5\ cm^{-3}$

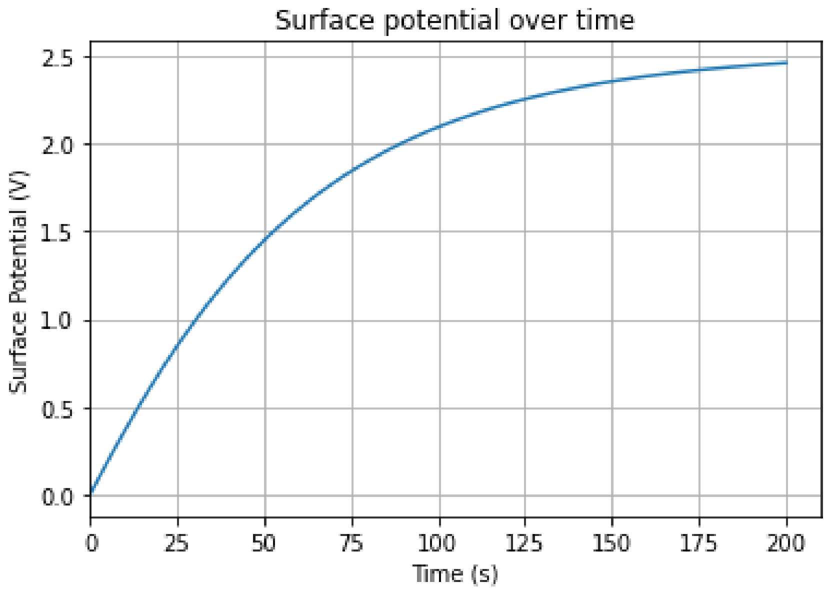


Figure 7: Evolution of the surface potential over time, T_e = 10 eV, n = 5 cm^{-3}

[Horanyi, 1989] [8] shows the evolution of the currents for specific inputs. One can use the program to find the same results from the article. Note that smaller grains will take much longer to reach equilibrium and the variations of the charge can be very small. When the size of the grain is changed, the time of simulation needs to be reconsidered.

4.5 Balance of the forces

The file is meant to compare the contributions of the different forces acting on the grain. To do so, we calculate the forces at a specific position (the initial conditions of position and velocities) and plot the magnitude of the forces for several sizes and masses of grain/debris. This allows us to look for the dominant force depending on the size and mass of the grain considered. In this section, the inputs related to the forces and the grain can impact a lot the results, as well as the initial conditions (example : distance from the earth, sun or comet). The program returns a plot with the magnitudes depending on the mass and radius.

Here's an example of the obtained results :

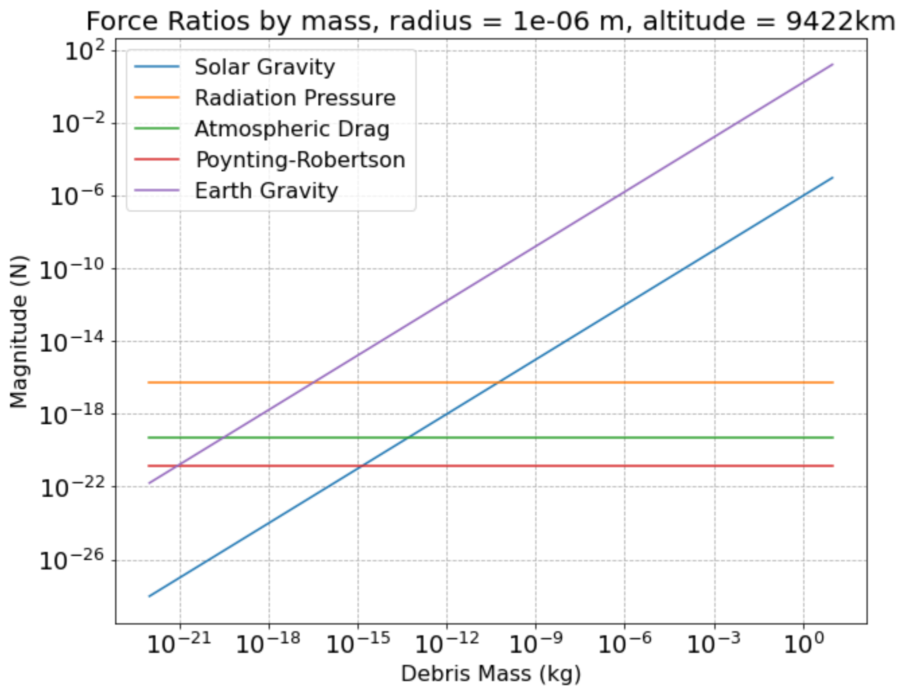


Figure 8: Balance of the forces acting on a grain as a function of the grain's mass

The figure above presents the contribution of the forces depending on the masses. Some of the forces do not depend on the mass, therefore its contribution remains constant. This is for the debris scenario. Other results can be found when running the script.

5 Perspectives

5.1 Limits of the model

The current model, while comprehensive, has several limitations that need addressing:

- **Simplistic Electromagnetic Model**: The model assumes a constant electromagnetic field, which is unrealistic for varying spatial conditions in both cometary and terrestrial environments.
- **Isotropic Charging Currents**: The model considers isotropic charging currents, not accounting for the directional nature of the photoelectric effect, which depends on the relative position of the dust grain or debris to the Sun.

- **Static Plasma Environment**: The plasma environment is assumed to be uniform and constant, neglecting the spatial and temporal variations that occur naturally.

- **Neglect of Inter-particle Coulomb Interactions**: The model does not consider the interactions between particles, which can become significant in dense environments.

- **Simplified Atmospheric Drag**: The atmospheric drag is considered constant, not taking into account the variations in density and temperature with altitude, which can significantly impact the dynamics of debris.

- **Computational Limitations**: The simulation time and step size are constrained, limiting the ability to simulate long-term dynamics and interactions over extended periods.

5.2 Suggestions to continue this work

To enhance the model and improve the accuracy of the results, the following suggestions are proposed:

- **Implement Spatially Varying Electromagnetic Models**: Develop and include an electromagnetic model that varies spatially to better represent the realistic conditions in space environments.

- **Directional Photoelectric Effect**: Modify the photoelectric current calculations to account for the directional nature based on the relative position to the Sun, improving the accuracy of charging predictions.

- **Dynamic Plasma Environment**: Introduce a dynamic plasma model that incorporates spatial and temporal variations in temperature and density, providing a more realistic representation of the plasma environment.

- **Inter-particle Coulomb Interactions**: Include the effects of Coulomb interactions between particles to account for collective behaviors and interactions in dense environments.

- **Variable Atmospheric Drag**: Implement an atmospheric model where density and temperature vary with altitude, significantly enhancing the accuracy of debris dynamics near Earth.

- **Optimize Computational Methods**: Explore and implement more efficient numerical methods and optimize the simulation code to handle longer simulation times and smaller time steps without compromising accuracy.

- **Realistic Initial Conditions**: Use realistic initial conditions for the positions and velocities of grains and debris, considering observational data and more accurate physical models to improve the predictive capabilities of the simulation.

- **Hybrid Numerical Methods**: Investigate hybrid numerical methods that combine the strengths of various algorithms to improve stability and accuracy in long-term simulations, especially for complex dynamical systems.

- **Optimize the Time of Simulation**: Specifically for debris, as one orbital period with a time step of 0.01 takes an important amount of simulation time (approximately 1 million steps depending on the altitude of the debris).

- **Improve 3D Representation**: The current representation is useful for visualizing trajectories, but the impact of the comet and Earth spheres is still not well understood. Additionally, the scales may not be adapted properly.
- **Consider Isotropic Charging Currents**: Currently, charging currents are considered isotropic, yet the photoelectric effect occurs when the dust grain or debris is exposed to sunlight. It would be interesting to vary the photoelectron current depending on the relative position of the grain to the Sun.
- **Dynamic Plasma Environment**: The plasma environment is also considered isotropic and very simplistic. Implementing a plasma model where the temperature and density of the species vary spatially would affect the Lorentz force, which could become more or less significant depending on the position of the grain.
- **Number of Grains in Simulation**: Considerations should be made about the number of grains in the simulation, as well as their respective positions. How far apart should they be ? Currently, the simulation considers random initial positions. With realistic models of atmosphere and electromagnetic fields, the trajectories of the debris or dust grains could vary significantly depending on the initial conditions.

By addressing these suggestions, the model can be significantly improved, leading to more accurate and reliable simulations of the dynamics of charged micro/nano dust and debris in various space environments. More references can be found in the other documents present in the folder.

References

[1] E. C. Whipple. Theory of the spherically symmetric photoelectron sheath' a thick sheath approximation and comparison with the ats 6 observation of a potential barrier. *Journal of Geophysical Research*, 81(4), 1976. Aeronomy Laboratory, Environmental Research Laboratories, NOAA, Boulder, Colorado 80302.

[2] Harold M. Mott-Smith and Irving Langmuir. The theory of collectors in gaseous discharges. *Physical Review*, 28(4):727, 1926.

[3] J. Allen, R. Boyd, and P. Reynolds. The collection of positive ions by a probe immersed in a plasma. *Proceedings of the Physical Society. Section B*, 70(3):297, 1957.

[4] M. J. M. Parrot, L. R. O. Storey, L. W. Parker, and J. G. Laframboise. Theory of cylindrical and spherical langmuir probes in the limit of vanishing debye number. *The Physics of Fluids*, 25(12):2388–2400, 1982.

[5] I. Mann, N. Meyer-Vernet, and A. Czechowski. Dust in the planetary system: Dust interactions in space plasmas of the solar system. *Physics reports*, 536(1):1–39, 2014.

[6] Mihály Horányi. Charged dust dynamics in the solar system. *Annual review of astronomy and astrophysics*, 34(1):383–418, 1996.

[7] Zhuang Liu, Dezhen Wang, and Gennady Miloshevsky. Simulation of dust grain charging under tokamak plasma conditions. *Nuclear Materials and Energy*, 12:530–535, 2017.

[8] M. Horányi. Charged dust in the earth's magnetosphere. In J. H. Waite, J. L. Burch, and R. L. Moore, editors, *Solar System Plasma Physics*. 1989.

[9] Jessica Agarwal, Yoonyoung Kim, Michael S. P. Kelley, and Raphael Marschall. Dust emission and dynamics. *arXiv preprint arXiv:2309.12759*, 2023.

[10] M. Horányi and D. A. Mendis. Trajectories of charged dust grains in the cometary environment. *The Astrophysical Journal*, 294:357–368, 1985.

[11] Antal Juhász and Mihály Horányi. Dynamics of charged space debris in the earth's plasma environment. *Journal of Geophysical Research: Space Physics*, 102(A4):7237–7246, 1997.

[12] Smriti Nandan Paul and Carolin Frueh. Space debris charging and its effect on orbit evolution. In *AIAA/AAS Astrodynamics Specialist Conference*, 2016.

[13] Dichotomy method. `http://encyclopediaofmath.org/index.php?title=Dichotomy_method&oldid=46648`.

[14] Runge-kutta methods. `https://en.wikipedia.org/wiki/Runge-Kutta_methods`.

[15] J. C. Butcher. *Numerical Methods for Ordinary Differential Equations*. J. Wiley, 2003. pp. 86–92.

[16] PlasmaPy Community. Plasmapy documentation: Boris algorithm. `https://docs.plasmapy.org/en/stable/api/plasmapy.simulation.particle_integrators.boris_push.html`, 2023. Accessed: 2024-06-27.

[17] Projects Publications Codes Courses Blog. Particle push in magnetic field (boris method). https://www.particleincell.com/2011/vxb-rotation/, 2011.