Design of a Quadrupole Mass

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The Designated 0roject *ommittee Approves the 0roject Titled

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By

Jorge)⸝ *ort+s

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A quadrupole mass spectrometer 8 as designed 8 ith the a ility to characteri9e the

tenuous atmosphere of Jupiter5s moon: Europa⸖ As a constraint: this instrument 8 as to fit

8 ithin a ; U cu esat chassis 8 ithout sacrificing measurement resolution and accuracy⸖)on

trajectories are studied through simulations carried out in the numerical computing

programming language: 3 AT , AB and the finite element analysis simulation soft 8 are:

*& 3 S&, 3 ultiphysics⸖ &ptimal mission parameters are then implemented in an

instrument design that 8 as uilt: tested: and validated⸖

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Figure #=A *loseꝹup of)on Trajectories
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Figure #>ᴀ Electric Ootential .enerated ʏ 2uadrupole
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3 otivation and Approach

The main motivation ehind this project is the spirit of discovery and eᴇploration Space eᴇploration is and 8ill al8ays e a domain of endless possi ilities)t is 8ith great motivation that) em ar ' on this journeyF a journey that 8ill hopefully ring a out insight to8ards methodologies used in discovering: eᴇploring: and characteri9ing strange: yet oddly familiar 8orlds The follo8ing encapsulates the project statement and approach

2uadrupole mass spectrometers are scientific instruments used in mass spectrometry: an analytical technique that uses the mass⅁to⅁charge ratio of an ion in order to identify its a undance 8ithin a given sample These types of instruments are used prevalently 8ithin the aerospace field 8here the main applications are in the study of planetary atmospheres and in monitoring the air quality during manned space missionsF the first of 8hich 8ill e dealt 8ith in this project

)n order to gain insight to8ards design parameters: a study 8ill first e conducted in modeling ion trajectories as they traverse a quadrupole mass spectrometer Equations of motion 8ill e derived and simulations 8ill e conducted &nce done: the design iteration process 8ill egin 8ith the goal of restricting the si9e to a ;U cu esat module G;"E#"E#" cmᴴ 8ithout affecting measurement resolution and accuracy A prototype of the quadrupole mass spectrometer 8ill then e uild in order to validate the design process

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!‰#   )ntroduction to , iterature - evie 8

The follo 8 ing literature revie 8 8 ill cover different articles concerning Europa 5 s

atmosphere: its surface composition: the Jovian magnetosphere: and the use of

via ility of organic life eEisting there҃ Although data regarding the surface or crustal composition is limited: the sputtered atmospheric constituents and nearDinfrared reflectance spectra of surface regions give a lot to study I<J҃ This data 8as gathered through the . alileo 1)3 S investigation҃ The 1ear)nfrared 3apping Spectrometer G1)3SH instrument had four main o jectives 8hen it 8as deployed on oard the . alileo &r iter I$JA

#҃ 3ap the distri ution of surface minerals on the . alilean satellites at spatial resolutions of $D;" 'm҃

!҃)dentify the phases and miEtures present thereon

;҃ *orrelate o served mineralogical distri utions 8ith the geomorphology o served 8ith the solidDstate imaging GSS)H system҃

<҃ Determine cloud morphology of the Jovian atmosphere and its structure over a 8ide range of phase angles҃

The data collected during the or it of the . alileo spacecraft a out Jupiter indicates that there are regions on Europa5s surface that demonstrate Ldistorted (⌐& vi rational overtone ands in the #҃$ and !҃" Mm regionN҃ This is particularly interesting ecause it indicates that these regions contain Lhighly concentrated solvated contaminantsN I<J҃)n order to understand the significance of this: one must first understand the term 0solvated5҃ Based off of the definition provided y the)nternational Union of 0ure and Applied *hemistry G)U0A*H: solvation is the process via 8hich a solute and a solvent ecome sta ili9ed҃ An eEample of this can e Lthe ionic groups of an ionDeEchange resinN I=J҃ This is a very strong indicator of radiolysis occurring on Europa5s surface҃ Although it

had een stated efore: the process of high energy particles disassociating surface

molecules as never proven to actually occur on Europa's surface. The data provided y

Figure 1: Sample Mass Spectrum Plot

Each peak corresponds to a specific molecular sample. The x-axis displays mass-to-charge ratio in increasing order and the y-axis depicts a relative intensity factor in increasing order. The highest peak, known as the base peak, is used as a reference to normalize the relative abundances of all the other ions present in the disassociated sample.

1.5.1 Quadrupole Mass Spectrometers

Quadrupole mass spectrometers are a specific type of mass spectrometer that are

;%;   )on Trajectories @ithin a 2uadrupole Field

The follo8ing is mostly a summary of the derivations found 8ithin Da8son5s Quadrupole Mass Spectrometry and Its Applications.

The electric field generated y the quadrupole rods is as follo8sᴧ

)t should e noted that there eEists a linear dependence on the coᴅordinate position᷼ From the equation: , , and   are 8eighting constants and E_o is ᴸa positionᴅindependent factor 8hich may e a function of timeᴺ I?Jᷓ Because the field is uncoupled in all three directions: the analysis of ion motion ecomes quite trivial᷼ &f course: this is assuming a perfect electric field᷼

,et us no8 consider the motion of an ion 8ithin this field᷼ Depending on the ion5s initial position: the force acting upon it varies᷼ The further the ion is displaced from the origin: the more it eEperiences the effects of the force: eE᷼)f 8e allo8 the field to follo8 restraints imposed y ,aplace5s equation: the follo8ing can e achieved᷼

To better comprehend the values assumed by x, y, and z the electric potentials should be solved for. Given that $-$: an integral may be carried out that would yield the following:

If we allow to equal $-$ and to equal 0 as it was previously stated: then the z term from the previous equation drops out and the eXpression becomes as seen below:

$$( )^{-}$$

As is analogous with potential flow theory pertaining to a fluid: this represents a field composed of equipotential lines as is shown in the figure.

Figure) Equipotential Lines for a Quadrupole Field

Four hyper olic cylinders produce these sets of equipotential lines: 8 here adjacent electrodes are oppositely charged. This is portrayed in figure S.

As seen a ove: the minimum distance et 8 een opposite electrodes is assigned the

term: $2r_o$⅜ @ith P Q ᴅ#ℝr_o! the electric potential   et 8 een the rods is given y the

eEpression   elo 8⅜

$$(\quad\quad\quad)$$

From here eEpression for the electric field in ~~the~~ and y direction can e o tained⅜

Attention is now turned towards obtaining the equations of motion. Let us start our motion analysis as with any other, considering Newton's Law.

From the Lorentz Force: we have the equation below, where e is the electric charge.

$$\vec{F} = e\vec{E} + e\left(\vec{v} \times \vec{B}\right)$$

This gives us the force due to an electric and magnetic field. We are only concerned with the force due to an electric field since quadrupole mass spectrometers are nonmagnetic instruments, therefore: our force equation becomes the below expression.

$$\vec{F} = e\vec{E}$$

We can thus rewrite Newton's Second Law as:

Utilizing the expressions formerly obtained describing the electric field in the x and y direction: the equations of ion motion become:

$$\left(\frac{e}{m r_0^2}\right)$$

Let us say ω_0 is constant and define the term A as seen below.

$$\left(\frac{e}{m r_0^2}\right)$$

The equations of motion are simplified to those seen here.

These are second order ordinary differential equations with the following solutions.

$$\sqrt{} \qquad \sqrt{}$$

$$\sqrt{} \quad \sqrt{}$$

The solution for $x(t)$ yields simple harmonic motion within the xz plane, $y(t)$ yields a "defocusing" within the yz plane.

The term n_o is not constant however. Instead, it is (usually) a periodic function as follows:

$$\left(\right) \left(\right)$$

$$\left(\right) \left(\right)$$

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<%#   !D Simulations Using 3 AT , AB

As a preliminary study: the equations of motion 8 ere modeled in 3 AT , AB5s Simulin ' tool oE% The loc ' diagram for the motion of an ion 8 ithin the CD4 plane of the instrument is seen elo 8 in figure >%

$igure 0% Simulin1 2 loc1 Diagram for Mathieu E*uation

These !D simulations 8 ill e eEpanded later% Trials 8 ill e reDdone and enchmar ' ed against pu lished data in order to validate the modeled equations% The results sho 8 n elo 8 are for an atomic mass of #= and ; !% The inscri ed radius: r_o: 8 as set as "%""$ mm and the voltage potentials 8 ere chosen to favor the ion of #= amu% As can e seen from figure B and ?: the ion of #= amu has oscillations ounded 8 ell 8 ithin the "%""$ mm

radius of the instrument while the ion of 21 amu oscillates well outside the boundary set by the inscribed radius.

Figure 8. Ion Oscillations Contained Within Instrument Bore Plane

Figure 9. Ion Oscillations Not Contained Within Instrument Bore Plane

<! ;D Simulations Using *& 3 S&, 3 ultiphysics

Simulations 8ithin *& 3 S&, are run 8ith the parameters sho8n in figure #" and the results can e seen in the follo8ing figures As 8ith the !D simulations: more cases 8ill e ran in order to conduct a parametric study and compare 8ith pu lished data

Name	Expression	Value	Description
r0	(2/768[mm]	0.002768 m	Rod radius
r0	re/1.1d	0.0024138 m	Inscribed radius
rsrc	0.75[mm]	7.57.3e-4 m	source radius
rcase	4*re	0.011072 m	Case radius
Lquad	1.7[m]/[mm]	... m	Quadrupole
a	0.05	0.05	Mathieu coe
q	...	...	Mathieu coefficie
f	4[MHz]	4E6 Hz	Frequency
omega	2*pi*f	2.5133E7 Hz	Angular frequen
mi	40[amu]	6.6422E-26 kg	Ion mass
Vac	q*mi*omega^2*r0^2/(4*e_const)	266.89 V	AC voltage
Udc	a*mi*omega^2*r0^2/(8*e_const)	0.5316 V	DC voltage
A	2[V]	2 V	Accelerating volt
v0	sqrt(2*e_const*A/mi)	3106.2 m/s	Initial x velocity

$igure "! &arameters ;sed for 'D Simulations
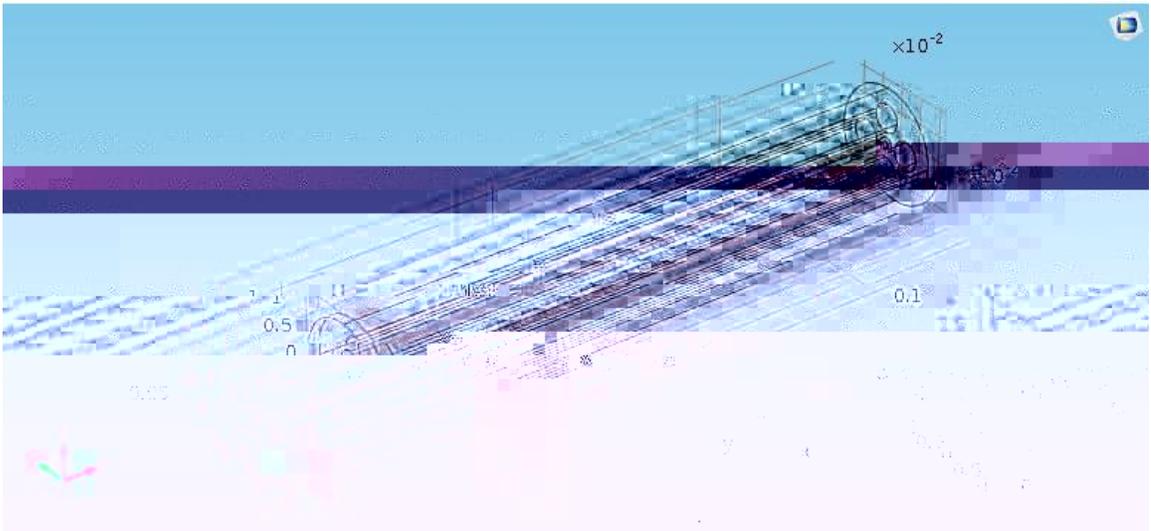
$igure ""% Quadrupole <eometr- in C4MS4+
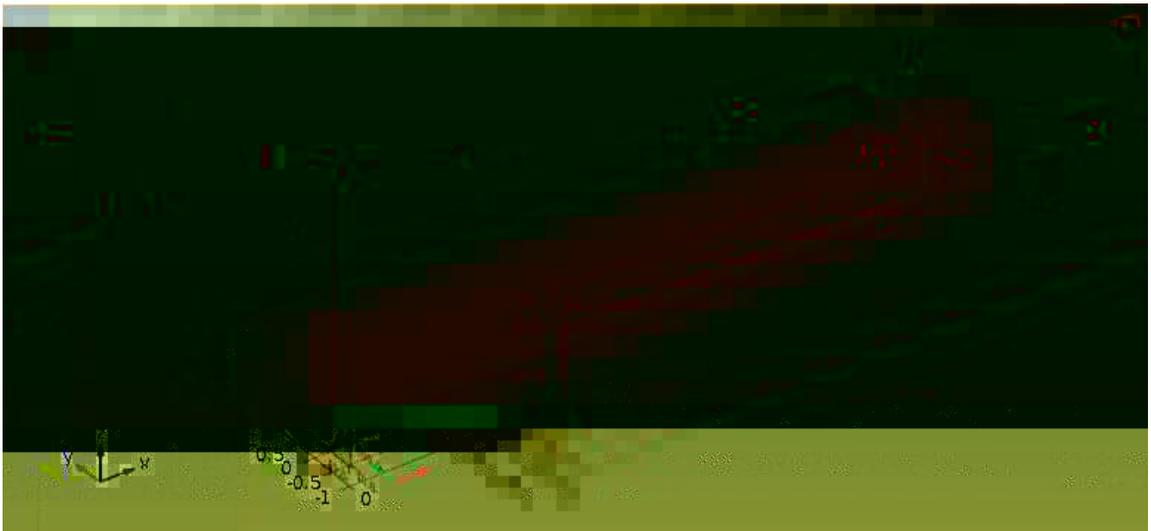
$igure " % Quadrupole Model in C4MS4+
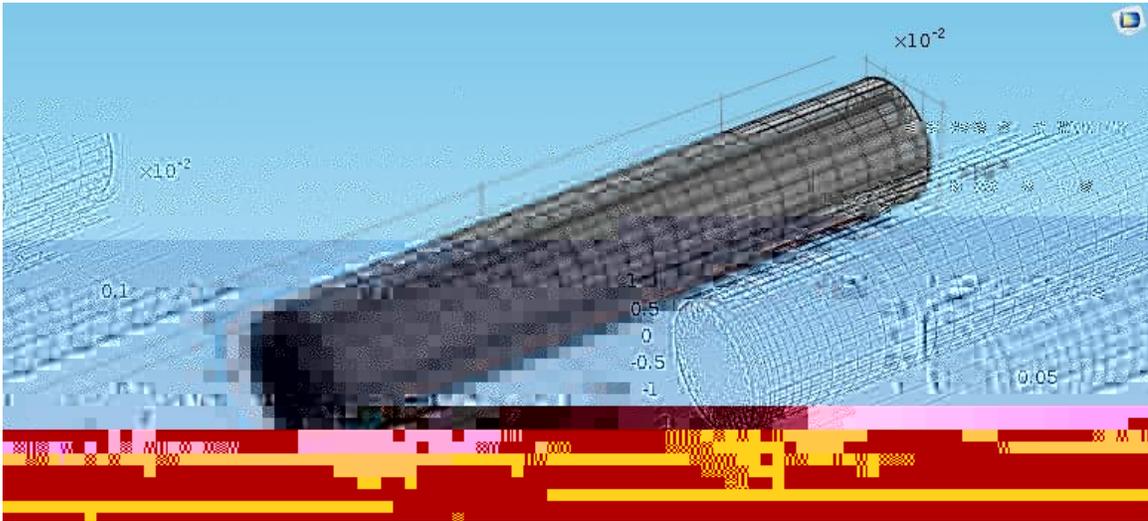
Figure 4.7: Mesh for Simulations
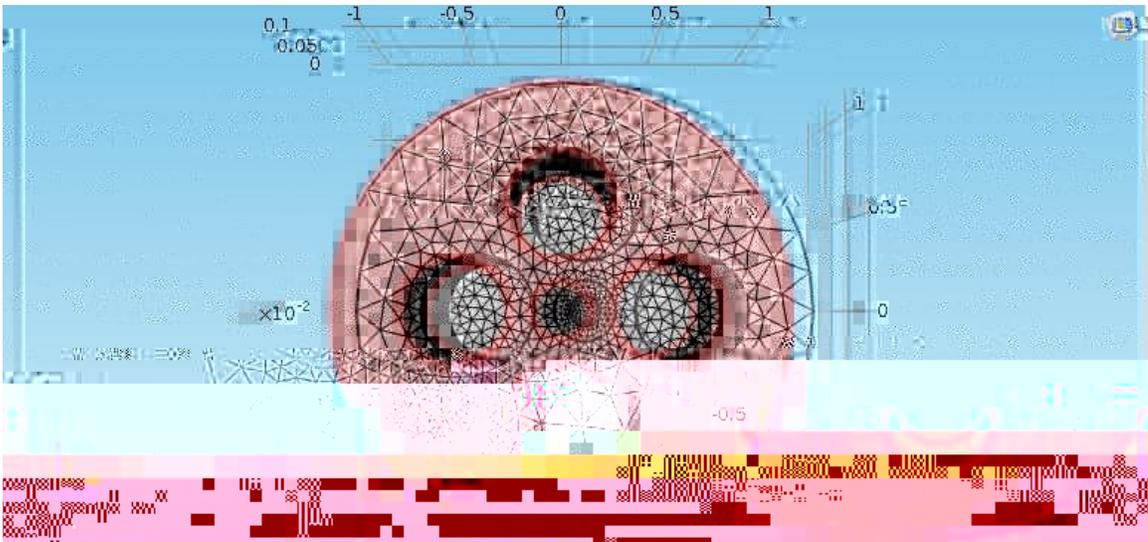
Figure 4.8: Free Triangular Mesh
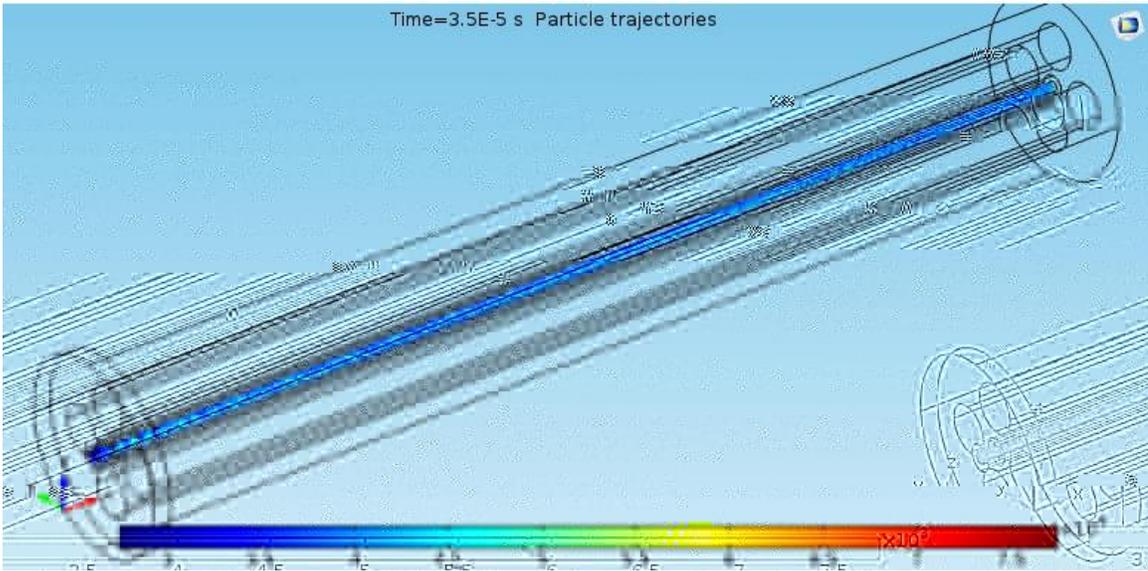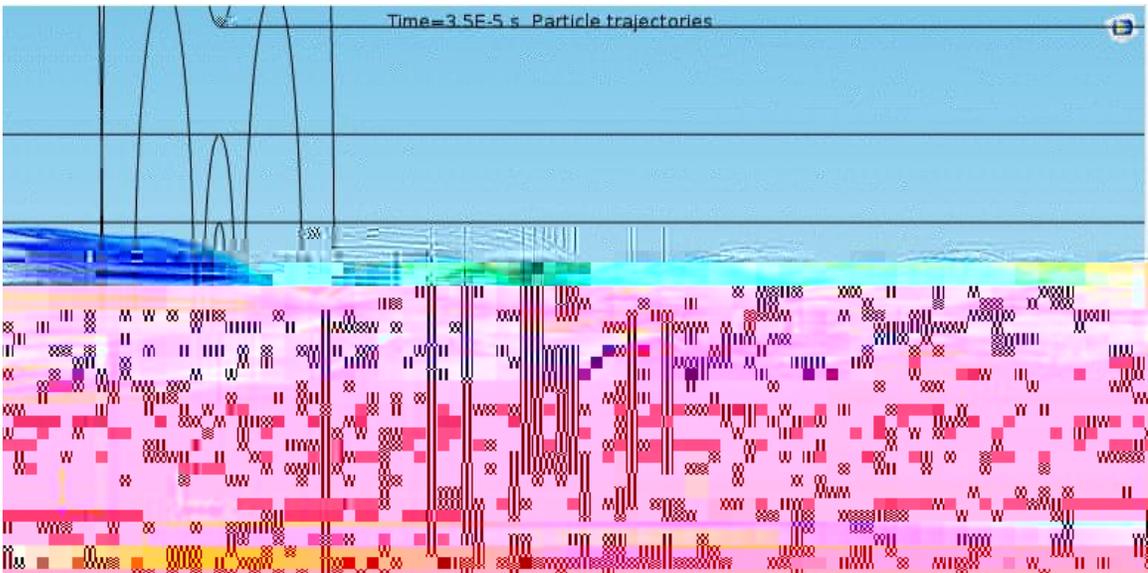
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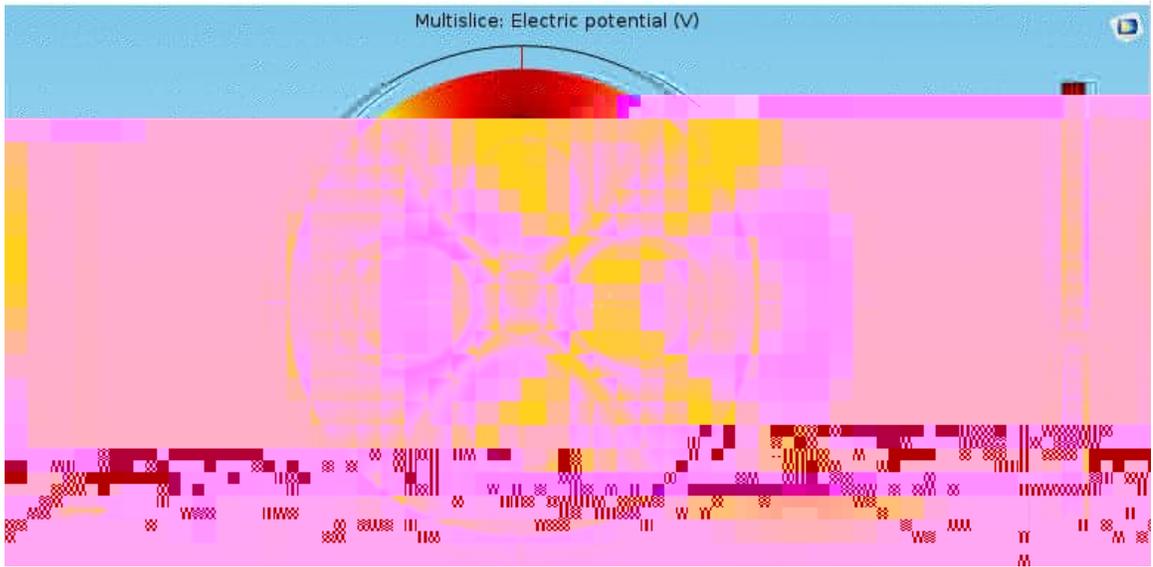
Johnson: -§ E§: , an9erotti: ,§ J§: S Bro8n: @§ ,§ G#?B!H§ 0lanetary applications of ion induced erosion of condensedDgas frosts§ *uclear Instruments and Met%ods in +%ysics , esearc%: ( ) -G#H: #<>D#$>§