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Fiscal Year:	FY 2023	Task Last Updated:	FY 03/20/2023
PI Name:	Gatsonis, Nikolaos Ph.D.		
Project Title:	Multiscale Computational Modeling of Dusty Plasmas Near Space Surfaces		
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Program/Discipline:			
Program/Discipline Element/Subdiscipline:	FUNDAMENTAL PHYSICSFundar	mental physics	
Joint Agency Name:		TechPort:	No
Human Research Program Elements:	None		
Human Research Program Risks:	None		
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Space Biology Cross-Element Discipline:	None		
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Comments:			
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No. of PhD Candidates:	1	No. of Master' Degrees:	0
No. of Master's Candidates:	1	No. of Bachelor's Degrees:	0
No. of Bachelor's Candidates:	0	Monitoring Center:	NASA JPL
Contact Monitor:	Callas, John	Contact Phone:	
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Flight Program:			
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Key Personnel Changes/Previous PI:			
COI Name (Institution):	Han, Daoru Ph.D. (University of Missouri, Rolla)		
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The goals of the proposed two-year research are to: develop and validate with Physical Sciences Informatics (PSI) data a state-of-the-art computational capability for modeling the release and transport of dust particles near floating and biased surfaces in space plasmas and use the multiscale capability and explore release and transport phenomena for spherical and non-spherical dust particles, under plasma and surface conditions beyond those addressed in the PSI experiment. The first objective is to develop a state-of-the-art dusty plasma computational modeling capability from the grain-scale to multiscale. The microscopic (grain-scale) Dusty Parallel Immersed Finite Element Particle-in-Cell (D-IFEPIC) model will be developed on the existing Parallel Immersed Finite Element Particle-in-Cell (PIFEPIC), a parallelized Particle-in-Cell (PIC) platform. The D-IFEPIC model will include spherical and non-spherical grains and will account for both surface and in-depth charging of each grain. D-IFEPIC will resolve the geometrical and material properties (permittivity) of each grain and model the unsteady and stochastic charging of grains via a deposition process. The multiscale Dusty Electrostatic Unstructured Particle-in-Cell with Collisions (D-EUPICC) model will be developed on the existing EUPICC, a parallelized hybrid PIC-Monte Carlo platform. The D-EUPICC model will include charging and transport of dust grains embedded into a plasma with electrons, ions, and neutrals. Forces on a grain will include gravity, Lorentz, Coulomb, neutral/ion drag, and adhesive van der Waals. The unsteady/stochastic charging of grains will be modeled with a multi-step Monte Carlo absorption collision with electrons and ions. The potential on a grain will be evaluated with a surface capacitance model. Electron motion will be integrated at inverse plasma frequency timesteps but ions and neutrals will use much larger timesteps following a sub-cycling scheme.

Task Description:

The second objective is to simulate the PSI experiment, validate the D-IFEPIC and D-EUPICC models, and quantify the plasma conditions under which the fluctuating charge on grains near a floating surface reaches a threshold such that the electric field force overcomes the adhesive van der Waals force. The two codes will be used with direct inputs from the PSI data and address comprehensively the multiscale interactions from grain-scale to system-scale observed in the PSI experiment.

The third objective is to use D-EUPICC and D-IFEPIC and investigate the parametric dependence of dust charging and release near floating and biased surfaces for a broad range of plasma and surface conditions beyond those found in the PSI experiment. These simulations will use spherical grains from 0.1-100 um and irregularly shaped grains (D-IFEPIC only), floating and biased surfaces in fully ionized plasmas found in low-Earth orbit (LEO), geosynchronous orbit (GEO), solar, and planetary environments. The results will document the dependence of charge and release time on these parameters and relative role of forces on grains. The comparisons will demonstrate the difference between the capacitance and the surface/in-depth charging models. The D-IFEPIC simulations with non-spherical grains will also demonstrate for the first time the impact of grain shape on sheath electrodynamics.

The proposed research directly addresses the scope of the solicitation: provides testing of hypothesis of dust charging and dust release mechanisms from surfaces in the PSI experiment; provides estimates of dust charging and release time for a wide range of grain sizes, surface potentials, and plasma conditions relevant to NASA missions using surface and surface/in-depth charging models; delivers an advanced modeling capability that can assist in the design of future ground-based and International Space Station (ISS)-based dusty plasma experiments as well, in the development of active methods for dust removal from extravehicular activity (EVA) suits or instruments exposed to plasmas; and enhances NASA's science readiness with the delivery of a validated capability for dusty plasmas that appear in broader areas of science and engineering.

Rationale for HRP Directed Research:

Research Impact/Earth Benefits:

The comparison with the PSI data allows validation of the multiscale modeling capability. The project entails use D-IFEPIC and D-EUPICC in an expanded parametric investigation of dust release for spherical and non-spherical grains under surface and background plasma conditions of interest to NASA beyond those in the PSI experiment.

Year 1 (10/2021-10/2022) efforts at Worcester Polytechnic Institute (WPI) and Missouri S&T (MST) addressed partially the three objectives of the study "Multiscale Computational Modeling of Dusty Plasmas Near Space Surfaces": 1. Develop a dusty plasma computational modeling capability from the grain-scale to multiscale 2. Simulate the PSI experiment of Flanagan and Goree (2006) and quantify the plasma conditions under which the fluctuating charge on grains near a floating surface reaches a threshold such that the electric field force overcomes the adhesive Van der Waals force. 3. Perform an expanded parametric investigation of dust release for spherical and non-spherical grains under surface and plasma conditions of interest to NASA beyond those in the PSI experiment. 1. Macroscopic Modeling of Surface Charging under Lunar Plasma Conditions with Implications to Dust Charging and Transport Progress at MST has been put towards modeling the macroscopic lunar surface charging as one of the main drivers of dust grain charging and transport which motivated the PSI experiment of Flanagan and Goree (2006). These simulations were performed with the MST-developed fully kinetic parallel immersed finite element particle-in-cell (PIFE-PIC) code which can resolve the uneven lunar surface terrain as well as landers and habitats on the surface of the Moon. Research for this task has been underway since October 2021 (concurrent with the NSTGRO project at MST). Particularly, this research considered the plasma charging near the lunar surface for future exploration missions, specifically, near lunar craters at the terminator region which are target destinations for planned Artemis missions. Under ambient solar wind and photoemission plasma conditions, the rugged surface terrain could generate localized plasma wakes and shadow regions which can lead to strong differential charging of the surface. Such localized plasma flow field together with the charged lunar surface provides an electric field leading to lofting and levitation of charged dust grains. In our study, the plasma species were chosen to include the ambient electrons and ions as well as photoelectron parameters at the lunar surface in the magnetosheath dayside environment (for which strong differential surface charging is expected). The environment's parameters were retrieved from NASA's Cross-Program Design Specification for Natural Environments (DSNE) document. The plasma conditions listed in the DSNE document include the mean, the 95% range, the 99.7% range, and the maximum range of the observed environments derived from the THEMIS-ARTEMIS data in the years 2012 through 2018. This study included the mean plasma conditions in the magnetosheath dayside environment, as well as the 99.7% range of the observed plasma conditions, which we will refer to as the "99.7%" plasma condition, in the magnetosheath dayside environment. This work has been accepted in February 2022 by the AIAA Journal of Space and Rockets (February 2023).

2. Microscopic Modeling of Irregularly Shaped Dust Grain Charging The team at MST also studied electrostatic interactions in dusty plasmas, particularly, charging of dust particulates in the collisionless regimes as the PSI experiment of Flanagan and Goree (2006). Considering the size of dust grains (order of microns) vs. the size of the glass

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Lask Progress: sphere (order of cm) used in the PSI experiment, the microscopic dust grain charging in the PSI experiment can be modeled as the configurations of dust grains near a "flat" surface, which were simulated using the PIFE-PIC code suite. A unique feature of our study is that both the permittivity and irregular shape of dust grains were explicitly resolved in PIFE-PIC. In this study, "irregular" shapes were achieved through patching of spheres. Multiple dust grain configurations were compared to see how dust grains are charged in stationary and drifting plasma environments. These included: single dust grain in a stationary plasma, multiple dust grains in a stationary plasma, multiple irregularly shaped dust grains in a stationary plasma, single/multiple dust grains in a drifting plasma, and single/multiple dust grains in a drifting plasma near a surface. Findings of this work has been presented at AIAA SciTech Forum 2023 as paper AIAA 2023-2616. These efforts made the PIFE-PIC code suite ready to model the Flanagan and Goree PSI experiment (2006) which is the focus of the ongoing effort. 3. Microscopic Modeling of Dust Charging and Comparisons with PSI Experiment Research during Year 1 at WPI focused on the development and implementation of a dust charging model to compare with the PSI experiment of Flanagan and Goree (2006) and Flanagan (2006). The dust in the PSI experiment was generated on a glass sphere immersed in a neutral neon gas and was found to be released when plasma was formed in the chamber due to the emission of an electron beam from a tungsten filament. Three cases were considered: Case a) involved dust charging in plasma with a cold and hot electron population. Case b) involved dust charging with the electron beam only. Case b) involved dust charging with the electron beam only. The dust charging model developed at WPI assumes an isolated spherical dust immersed in a stationary plasma and is implemented numerically. The dust charging model computes the time-dependent charge on the dust, calculated using an isolated capacitor model. The simulations assume that micron-sized particles are adhered to a dielectric surface (glass sphere) and exposed to the conditions for Case a) and Case c) from the PSI experiment. Case b) of the PSI experiment did not provide enough experimental data for numerical analysis. The simulations provide the charge acquired by the dust particle and the floating potential, and used to predict the electric force on the dust using the electric field evaluated from the PSI experiment. This electric force is then compared to the Van der Waals adhesive force on the dust and the conditions for particle release are determined at the time when the electric force is larger than the Van der Wall. Simulation results from the isolated dust model show that the dust is released under certain plasma and beam conditions in accordance with the PSI experiment. Ongoing particle-in-cell (PIC) simulations of isolated dust particles are validated with this theoretical model. Additional fully 3D PIC simulations of layers of spherical dust particles adhered to the dielectric glass surface will be performed in Year 2 and results will be compared directly with the PSI experiment **Bibliography Type:** Description: (Last Updated: 03/20/2023) Lund, D., He, X. Han, D. "Kinetic Particle Simulations of Plasma Charging at Lunar Craters Under Severe Conditions" Abstracts for Journals and Journal of Spacecraft and Rockets, AIAA **Proceedings** https://doi.org/10.2514/1.A35622, Jan-2023 Lund, D. and Han, D. "Kinetic Particle Simulations of Charging of Irregularly-Shaped Dust Grains in Low Temperature Abstracts for Journals and Collisionless Plasmas" 49th International Conference on Plasma Science (ICOPS 2022), Seattle, Washington, USA, May **Proceedings** 49th International Conference on Plasma Science (ICOPS 2022), May-2022 Han, D., Jianxun Zhao, J. and Lund, D. "Kinetic Particle Simulations of Plasma Charging and Dust Transport near the Abstracts for Journals and Lunar Terminator" 32nd International Symposium on Rarefied Gas Dynamics (RGD32), Seoul, South Korea and **Proceedings** Virtual, July 4-8, 2022 32nd International Symposium on Rarefied Gas Dynamics (RGD32), Jul-2022 Lund, D. and Han, D. "Kinetic Simulations of Charging of Irregularly-Shaped Dust Grains in Space Plasmas" The 7th Abstracts for Journals and Annual Meeting of SIAM Central States Section, Stillwater, OK, October 1-2 2022

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