Novel approaches to multiscale geospace particle transfer:

Improved understanding and prediction through uncertainty quantification and machine learning

Executive Summary

The magnetosphere, ionosphere and thermosphere (MIT) act as a coherently integrated system (geospace), driven in part by solar influences and characterized by variability and complexity. The manifestation of this variability and complexity is known as space weather, which refers to the effects of solar energy in geospace that threaten the technological infrastructure that powers the world [*Schrijver et al.*, 2015]. Space weather events also known as "geomagnetic storms" can disrupt the operation of power grids, magnetic surveying and directional drilling for oil and gas. These storms also heat the ionosphere-thermosphere (~100-1000 km altitude), changing density and composition and disrupting radio communications and Global Navigation Satellite Systems (GNSS). Storm-driven charged particles and radiation throughout geospace are a hazard to the health of astronauts, passengers on high altitude flights and all space-based technologies.

Among the most important and yet uncertain aspects of the geospace system is energy and momentum coupling between regions, which is accomplished by electromagnetic fields, or Poynting flux, and the transfer of charged particles. Particles are transferred from the magnetosphere to the ionosphere in a process known as particle precipitation [e.g., *Hardy et al.*, 1985], and particles of ionospheric origin undergo energization to escape to the magnetosphere [e.g., *Strangeway et al.*, 2000]. Flow of particles in both directions are critical to the composition and dynamics of each region and are inherently multiscale processes. However, existing models do not capture the multiscale aspects, largely neither address nor quantify uncertainties, and are increasingly ill-equipped to provide the specification necessary for the growing demand for space weather forecasts. ***The extent to which shortcomings in existing models of particle precipitation and ion outflow impact our understanding of geospace and ability to predict space weather is unknown.***

Due to recent trends in the availability of data, we now face an exciting opportunity to progress geospace understanding through the intersection of traditional approaches and state-of-the-art data-driven sciences [McGranaghan et al., 2017]. Data (from simulations and direct observations distributed throughout the solar wind and geospace system) are now available to take advantage of cutting-edge data-driven approaches, summarily referred to here as 'machine learning' (ML) techniques. Although Poynting flux can be quantified at large scales via global observations of ionospheric convection (e.g., from the Super Dual Auroral Radar Network, SuperDARN) and field-aligned currents (e.g., from the Active Magnetosphere and Planetary Electrodynamics Response Experiment, AMPERE) [*Waters et al.*, 2004], comparable global observations of particle transfer are not available. We propose a workshop that will cut across disciplinary lines to better utilize particle transport data for the prediction of energy and momentum transfer in geospace by the ML techniques of uncertainty quantification and neural networks. The proposed work will produce a leap forward in the understanding of geospace particle transfer, both in the quantification of the uncertainties of current models (e.g., data products that quantify how unknowns in electron particle precipitation map to errors in ionospheric conductivity estimation on different scales) and by establishing a foundation for improved predictive models using neural networks.

1. Science Rationale

1.1: Questions

We propose to address the following questions:

1. What are the quantitative uncertainties in (existing) particle precipitation and ion outflow models?
2. To what extent do these uncertainties propagate to uncertainties in critical space weather parameters of the magnetosphere and ionosphere (e.g., magnetospheric composition and ionospheric conductivity)?
3. To what extent can neural networks yield improved models of particle precipitation and ion outflow, and, ultimately, improve space weather forecasts?

1.2 Background

Critical variables for space weather are the flux distribution of electrons precipitating into the high-latitude ionosphere and their integrated hemispheric precipitation rates and power [*Zhang et al.*, 2015]. Global simulations of geospace include either index-based, empirical precipitation models [*Ridley et al.*, 2006; *Codrescu et al.*, 2012; *Qian et al.*, 2014], or simple first-principles causal models [e.g., *Wiltberger et al.*, 2009]. All of the existing simulation models of electron precipitation exhibit deficiencies either in causal regulation, neglect of key types of precipitation, or accuracy and scales [*Zhang et al.*, 2015].

When the ionosphere is heated by any number of processes, including particle precipitation, Joule heating, and photoionization [*Burns et al.*, 2007], cold ionospheric O^+ particles are accelerated upwards in altitude. With sufficient acceleration, these particles escape to the magnetosphere in a process known as ion outflow. Outflow has been shown to occur at all local times at mid- and high-latitudes [*Loranc et al.*, 1991], forms a dominant source of magnetospheric plasma [*Yau et al.*, 1997], and leads to temporal and spatial variations in magnetospheric composition, Alfvén speed, and ring current pressure distribution [*Redmon et al.*, 2014]. Like particle precipitation, modeling of ion outflow has taken several forms, including ad hoc [*Zhang et al.*, 2007], empirical [*Strangeway et al.*, 2000], and simplified physics-based [*Glocer et al.*, 2009; *Varney et al.*, 2016] approaches. None of the existing models sufficiently address the numerous complex driving processes.

Remedying shortcomings in the specification of particle transport between the magnetosphere and ionosphere is critical. The movement of particles affects the composition and dynamics of both regions. In the ionosphere precipitating particles collide with ambient particles, driving ionization which alters the conductivity, and hence the ionospheric electrodynamics, and creating ionospheric irregularities which threaten the integrity of radio communication [*Kintner et al.*, 2007]. Ion outflow changes composition and pressure distributions in the ionosphere and the magnetosphere [*Glocer et al.*, 2009]. Both precipitation and outflow affect the neutral density environment, a critical uncertainty for satellite and orbital debris drag estimation [*Marcos et al.*, 2006]. ***With the increased accessibility of data with which to study the coupled geospace environment, we can now explore particle transport through multidisciplinary data-driven approaches. This project will be a demonstration of the potential for uncertainty quantification and neural network techniques to provide a significant leap forward in the understanding, and, ultimately, prediction of the transfer of particles in geospace.***

2. Methodology

2.1 Principal Objectives:

We will address two specific tasks:

1. Assess the impact of uncertainties in specification of electron precipitation and ion outflow on the MIT system (model-driven)
2. Explore neural network models to improve specification of electron precipitation and ion outflow (observationally-driven)

2.2 Task One: Assess the impact of electron precipitation and ion outflow on simulations of the ionosphere, magnetosphere, and radiation belts

The first task will be to quantify the uncertainties of magnetosphere and ionosphere models to electron precipitation and ion outflow. Team co-leader Camporeale outlined the approach that we will use in the context of radiation belt simulations. Namely, they propagated uncertainties originating from specific radiation belt model input parameters through the nonlinear simulation and quantified the resultant variability using an ensemble of simulations. Their work produced actionable new understanding to improve space weather predictions associated with the radiation belts. This project will take advantage of their pioneering work to produce similar new understanding for the geospace phenomena influenced by electron precipitation and ion outflow. We will examine the Global Ionosphere-Thermosphere Model (GITM) [*Ridley et al.*, 2006] and the Lyon-Fedder-Mobarry (LFM) model [*Lyon et al.*, 2004] to simulate the ionosphere and the magnetosphere, respectively. Because the radiation belts are integrally connected to particle transport, we will also assess the effects in radiation belt simulations using the Versatile Electron Radiation Belt (VERB) Model [*Shprits et al.*, 2008]. Each of these models are chosen based on extensive benchmarking, wide acceptance, and direct expertise on our team.

To conduct the uncertainty quantification two steps must be taken: 1) determine the range of electron precipitation and ion outflow inputs to the simulations based on the variability of existing models and 2) run the ionosphere, magnetosphere, and radiation belt models for the range of input conditions thereby propagating the uncertainties through the simulations. The range of electron precipitation and ion outflow inputs will be determined from the Oval Variation, Assessment, Tracking, Intensity, and Online Nowcasting (OVATION) Prime [*Newell et al.*, 2010] and the Ionosphere Polar Wind Model (IPWM) [*Varney et al.*, 2016] models, respectively. We note that there may be computational limitations to running these complex models across the range of inputs and acknowledge that our workshop may rely on simplified, or surrogate, versions of the models. All models that will be used for task one can be run on-demand at the Community Coordinated Modeling Center (CCMC, https://ccmc.gsfc.nasa.gov/) and their results archived so that the data are freely and openly available to the entire community. Therefore, our work will provide benefit to the community beyond the conclusion of the proposed workshop.

2.3 Task Two: Explore machine learning models to develop improved particle precipitation and ion outflow specification

The second task will be to provide the first exploration of the efficacy of neural network-based ML models to specify electron precipitation and ion outflow. The objective of the ML models will be to determine statistical relationships between solar wind drivers and geomagnetic activity parameters and electron precipitation and ion outflow that could improve accuracies of ionosphere and magnetosphere models. We will focus on neural networks with deep architectures, given recent breakthroughs using this approach [e.g., *Krizhevsky et al.*, 2017] and demonstrated potential for geospace [*Bortnik et al.*, 2016]. Deep neural networks have the ability to learn complex statistical relationships [*Lecun et al.*, 2015], and, therefore, have the potential to progress the modeling and prediction of particle transport in geospace. Finally, we will place emphasis on recurrent neural networks (RNN), specifically Long Short-Term Memory (LSTM) [Hochreiter and Schmidhuber, 1997], as the current state-of-the-art for sequential data and for systems that exhibit `memory', or hysteresis [*Cho et al.*, 2014]. ***RNNs are largely unexplored for geospace applications.*** Using input data from the solar wind, geomagnetic activity indices (e.g., the auroral electrojet index (AE)), and geospace observations we will investigate the use of RNNs to discover relationships with the following output data:

1. electron precipitation data from the Defense Meteorological Satellite Program (DMSP) spacecraft; and
2. ion outflow data as measured by the DMSP and Fast Auroral SnapshoT (FAST) Explorer spacecraft.

McGranaghan et al., [2016] demonstrated the immense information content of DMSP particle precipitation data to inform advanced methods to specify and characterize the electron flux environment. Likewise, similar benefit of data-driven methods has been realized for ion outflow using DMSP [*Coley et al.*, 2003] and FAST [*McFadden et al.*, 2013] observations. Appendix A.1 details the project data sets and their availability for this work. These data sets will compose capable training and testing databases for RNN exploration.

3. Unique Team Composition

Our outstanding international team has been uniquely constructed for the multidisciplinary needs of this ambitious project. We have appointed leads for each of the core competencies of the project (see Table 1). In addition to core members, we have identified external ML advisors and an early career scientist to enhance our capability to bring closure to the project goals. External ML experts will contribute on a consultant-basis and early career scientist and pioneer of ML methods in geospace [*Zhelavskaya et al.*, 2016] Irina Zhelavskaya has committed to a role equivalent to the core team.

Table 1: Project team and core competencies*†

Member	**Project core competency lead area**	**Affiliation**	**Country**
Ryan McGranaghan	Team co-leader	NASA Jet Propulsion Laboratory/National Center for Atmospheric Research (NCAR)	USA
Enrico Camporeale	Team co-leader	Centrum Wiskunde & Informatica, Amsterdam	NLD
Binzheng Zhang	Ion outflow	University of Hong Kong	CHN
Jesper Gjerloev	Particle precipitation	Johns Hopkins University Applied Physics Laboratory/University of Bergen	USA/NOR
Kristina Lynch	Ionospheric system	Dartmouth College	USA
Susan Skone	Ionospheric impacts	University of Calgary	CAN
Yuri Shprits	Magnetospheric system	The Helmholtz Centre Potsdam - GFZ	DEU
Mick Denton	Magnetospheric impacts	Space Science Institute	USA/GBR
Alison Lowndes	Machine learning and computation	Artificial Intelligence DevRel | EMEA | NVIDIA Ltd	GBR
Peter Riley	Uncertainty Quantification	Predictive Science Inc.	USA
Irina Zhelavskaya	Early career	The Helmholtz Centre Potsdam - GFZ	DEU

*Each member of the core team will serve as a 'lead' of one aspect of the problem.

†Each team member has demonstrated leadership and expertise in novel methods for space science

4. Expected Outcomes

Anticipated innovations include quantitative evaluation of the uncertainties of existing electron precipitation (i.e., OVATION Prime) and ion outflow (i.e., IPWM) models and new neural network-based models for these phenomena. We expect to:

- Pioneer new collaborations between heliophysics and machine learning communities;
- Produce publications in both space physics- and machine learning-focused journals (target two major publications with all team members as co-authors: one in space physics journal and one in machine learning journal); and
- Disseminate results at conferences with corresponding conference publications.

Our efforts will enhance the infrastructure for space science discovery by fostering partnerships between science and ML communities and demonstrating the value of neural network approaches for space science. Our data and code will be made freely and openly available to ensure that future efforts can build on our progress. Finally, we will culminate our work in a final report, detailing our approach, progress, and targeted future work.

5. Meeting Structure and Timeline

We propose two week-long meetings at ISSI-Bern over a 12-month period. The meetings will occur in the Fall of 2018 and Spring of 2019, respectively. Working groups will be formed at the start of the first meeting to facilitate concurrent progress toward both project tasks at each meeting. Between meetings, and to prepare for publications and conference dissemination of our results, we will hold regular team virtual meetings.

6. Facilities and Financial Support/Feasibility

The standard package for support provided by ISSI, including support for our team meetings, projection and meeting technologies, and internet access, will be sufficient for our project. If travel funding for only one team leader is available, co-leader Camporeale can renounce travel funding. We intend to utilize the added 15-20% of the total grant to bring in Irina Zhelavskaya as an early career scientist.

7. Added Value of ISSI

This ambitious project requires rapid progress and a broad range of expertise, covering space science, space weather, machine learning, and data science. This environment is uniquely provided by ISSI. Involvement with ISSI will allow us to take advantage of relevant previous and ongoing ISSI workshop teams, notably “Determination of the Global Conductance Pattern and its Influence on the Dynamics of Geospace” and “Multi-Scale Variations in Auroral Electron Precipitation.” Likewise, our workshop would enrich the ISSI community, being the only recent effort to study geospace through ML approaches.

Appendices

A.1: Project data sets

Neural network input data (predictive variables)		
Data set	**Team member(s) with relevant expertise**	**Data access**
Solar wind data and geomagnetic activity indices	All	https://omniweb.gsfc.nasa.gov/
Swarm	McGranaghan	https://earth.esa.int/web/guest/swarm/data-access
Super Dual Auroral Radar Network (SuperDARN)	Lynch, Gjerloev	http://vt.superdarn.org/tiki-index.php
Super Magnetometer Initiative (SuperMAG)	Gjerloev	http://supermag.jhuapl.edu/
Advanced Magnetosphere and Planetary Electrodynamics Response Experiment (AMPERE))	Gjerloev, McGranaghan	http://ampere.jhuapl.edu/
Ionospheric data from Global Navigation Satellite Systems (GNSS) signals	Skone, McGranaghan	*Numerous sources*
Van Allen Probes	Shprits, Denton, Camporeale, Zhelavskaya	http://vanallenprobes.jhuapl.edu/
Neural network output data (predicted variables)		
Data set	**Team member(s) with relevant expertise**	**Data access**
Defense Meteorological Satellite Program (DMSP) particle data	Gjerloev, McGranaghan	https://www.ngdc.noaa.gov/stp/satellite/dmsp/
Fast Auroral SnapshoT (FAST) Explorer particle data	Zhang, McGranaghan	http://sprg.ssl.berkeley.edu/fast/
Solar wind data and geomagnetic activity indices	All	https://omniweb.gsfc.nasa.gov/

A.2 Team information

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Dr. Ryan McGranaghan takes a multi-disciplinary approach to the study of space science, bringing together traditional space physics with innovation from the field of data science. His passion for data-driven discovery has led to involvement in the JPL Data Science Working Group, the NASA Frontier Development Lab artificial intelligence R&D incubator, and complex systems institutes throughout the United States. In addition to providing team leadership and coordination, Ryan will contribute to accessing, mining, and analyzing the numerous data sources involved in the proposed work, formulating the machine learning problem and creating actionable data products from the uncertainty quantification and neural network tasks. He will also provide expertise in particle precipitation, magnetosphere-ionosphere coupling, and space weather.

Dr. Enrico Camporeale has a broad expertise in Space Plasma, Numerical Methods and Machine Learning. He is leading a project on real-time forecasting for killer electrons in the radiation belts using Machine Learning at the Dutch National Center for Mathematics and Computer Science (CWI) and actively working on several aspects of using Deep Neural Networks for Space Weather prediction. He is an associate editor of the Journal of Space Weather and Space Climate. He will contribute in defining and tailoring Machine Learning algorithms to the space weather forecasting problem.

Dr. Binzheng Zheng has expertise in modeling space plasma physics, with a focus on system-level studies of the interaction between the solar wind, magnetosphere, ionosphere and upper atmosphere, including neutral dynamics, plasma electrodynamics, magnetohydrodynamics (MHD), and collisionless transport processes. As a member of the LTR (LFM-TIEGCM-RCM) model development team, he has extensive experience in advancing the particle precipitation model and implementing ionospheric outflow models in the magnetosphere-ionosphere (M-I) coupling process. He will contribute to exploring/incorporating the multi-scale particle transport process in high-resolution, coupled global-scale geospace simulations.

Dr. Jesper Gjerloev is currently Principle Professional Staff scientist at Johns Hopkins University - Applied Physics Laboratory in Laurel, Maryland. He is world-wide recognized scientists studying Earth - near Space interactions. He received his master degree from the Niels Bohr Institute (theoretical space plasma physics) and his PhD in space physics (auroral electrodynamics) from Danish Technical University while performing the research at NASA - Goddard Space Flight Center. He has been involved in numerous large projects including the ACES rocket experiments, the SuperMAG collaboration, the ARCH project, and the Birkeland mission (serving as the PI of the last three projects).

Dr. Kristina Lynch studies the plasma physics of the auroral ionosphere, using sounding rocket investigations from Alaska and Norway. Her research interests right now focus on gathering together observations from a variety of sources (in situ, groundbased imagery, radars) at a variety of scale sizes to build an integrated picture of the ionospheric signatures of auroral structures. Her students are presently working to use machine learning techniques in combining auroral imagery with in situ and radar field information. She is a Professor of Physics and Astronomy at Dartmouth College. She brings to this project a specific and active interest in these techniques as applied to the auroralionosphere.

Dr. Susan Skone has 25 years of experience leading more than 30 sponsored projects investigating space weather phenomena, associated impact on satellite-based navigation systems, and improved positioning/navigation methods for aviation, marine and land applications. She is primary developer of licensed software tools for ionospheric remote sensing using GNSS signals (TECANALYS, TECMODEL) and has developed a full suite of hardware and software simulator tools, software receivers, instruments and models for GNSS analysis. Susan will contribute to GNSS data processing and characterization of key space weather impact parameters.

Dr. Yuri Shprits is head of the section "Magnetospheric Physics" at GFZ Potsdam. His primary area of scientific research is understanding the dynamics of the radiation belts and their effect on satellites, through data analyses, modelling and data assimilation. He is a member of the editorial board of ELSEVIER Space Science Reviews Journal (since 2012), Vice-chair of COSPAR sub-committee D3.3, Member of the UCAR Jack Eddie Fellowship steering committee (2013- 2016), and is an awardee of the Presidential Early Career Award for Scientists and Engineers (2012). His contribution will be to assess the effects of particle transport in radiation belt simulations using the Versatile Electron Radiation Belt (VERB) Model.

Dr. Mick Denton's research efforts are driven by a desire to understand the physical mechanisms at work in the solar-terrestrial environment. He has a broad range of modelling and data-analysis expertise. Recent research has focused on (i) the composition within Earth's radiation belts and plasma sheet, (ii) refilling processes in the ionosphere/plasmasphere, and (iii) empirical forecasting of particle populations in the inner magnetosphere.

Alison Lowndes: After spending her first year with NVIDIA as a Deep Learning Solutions Architect, Alison is now responsible for NVIDIA's Artificial Intelligence Developer Relations in the EMEA region. She is a mature graduate in Artificial Intelligence combining technical and theoretical computer science with a physics background & over 20 years of experience in international project management, entrepreneurial activities and the internet. She consults on a wide range of AI applications, including planetary defence with NASA & the SETI Institute and continues to manage the community of AI & Machine Learning researchers around the world, remaining knowledgeable in state of the art across all areas of research. She also travels, advises on & teaches NVIDIA's GPU Computing platform, around the globe. Twitter: @AlisonBLowndes.

Dr. Peter Riley is a Senior Scientist at Predictive Science Inc. (PSI) . He has more than 20 years' research experience both in the analysis of complex datasets and the development and implementation of massively parallel computational algorithms, particularly in Heliophysics. He leads and/or has led a number of NASA, DoD (DTRA, NCMI, Air Force, NRL), and NSF efforts involving mathematical modeling and high performance computing and has developed and delivered real-time algorithms to NOAA. He is an instrument team member for several NASA spacecraft missions and currently serves, has served on a number of NASA and NSF working groups and steering committees. Dr. Riley's current research focuses on analysis and modeling of complex systems ranging from solar physics to infectious diseases.

Irina Zhelavskaya has expertise in Data Analysis, Machine Learning, and Magnetospheric Physics. She is currently pursuing PhD in Magnetospheric Physics at GFZ Potsdam where she uses neural networks to quantify the dynamics of cold plasma in the plasmasphere. Prior to the work in Magnetospheric Physics, she was majoring in Computer Science, and received MSc in Computer Science (honours) from Skoltech, Russia, in close collaboration with MIT where she spent 1,5 years. During her MSc thesis she worked on applying machine learning techniques to satellite data and building predictive data-driven models. Irina will contribute to development and implementation of the Machine Learning algorithms for space weather forecasting.

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