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Abstract

Predicting variations in the near-Earth space environment that can lead to spacecraft damage and failure, i.e. "space weather", remains a big space physics challenge. A new capability was developed at Los Alamos National Laboratory (LANL) to understand, model, and predict Space Hazards Induced near Earth by Large Dynamic Storms, the SHIELDS framework. This framework simulates the dynamics of the Surface Charging Environment (SCE), the hot (keV) electrons representing the source and seed populations for the radiation belts, on both macro- and micro-scale. In addition to using physics-based models (like RAM-SCB, BATS-R-US, and iPIC3D), new data assimilation techniques employing data from LANL instruments on the Van Allen Probes and geosynchronous satellites were developed. An order of magnitude improvement in the accuracy in the simulation of the spacecraft surface charging environment was thus obtained. SHIELDS also includes a post-processing tool designed to calculate the surface charging for specific spacecraft geometry using the Curvilinear Particle-In-Cell (CPIC) code and to evaluate anomalies' relation to SCE dynamics. Such diagnostics is critically important when performing forensic analyses of space-system failures.

Background and Research Objectives

Our society is increasingly dependent on satellite-based technologies (broadcast TV/Radio, cell phones, GPS, internet, commercial/military/national security assets) susceptible to harmful conditions in space, i.e. "space weather" [1]. As satellites orbit around the planet, they are bombarded with charged particles, and surface charging results from the collection of charged particles by the spacecraft. Surface charging can lead to potential differences across spacecraft components and cause discharges that can damage electronics [2]. The primary source of the spacecraft Surface Charging Environment (SCE) is the hot (~10's keV$\approx 10^8$ K) electrons [3] injected from the magnetotail into the inner magnetosphere during storms and substorms. These space weather events [4, 5] are triggered by plasma eruptions on the Sun slamming into Earth 1 to 4 days later. Storms intensify the ring current, the magnetically trapped charged particles (~1- 100 keV) circling Earth between ~2 to 5 Earth radii (R_E). Dramatic magnetospheric disruptions called "substorms" wherein the nightside magnetosphere reconfigures on a timescale of minutes, occur several times per day, releasing fast plasma flows and injecting hot electrons into the near-Earth region. Due to missing processes and lack of coupling at the relevant scales, accurate specification of the SCE by state-of-the-art space weather models at any given time and location, has been challenging. One of the major objectives of SHIELDS was to better understand storm/substorm injections, their magnitude and depth of penetration, and the subsequent evolution of the injected particles responsible for the SCE.

Furthermore, an important consequence of particle injections is the generation of plasma waves which transfer energy from the fields back to the particles. Like a surfer riding an ocean wave, charged particles can be pumped to very high energies becoming "killer electrons" that damage spacecraft, or can be precipitated (lost) into the Earth's atmosphere producing the spectacular aurora. This extremely complex feedback mechanism regulates the intensity and distribution of particle populations as a delicate balance between sources and losses. How the competing acceleration and loss processes operate to produce these populations has been one of the longest-standing unresolved problems in space research since the discovery of the radiation belts [6] by Van Allen in 1958. It was long thought that radial transport from an outside source was the dominant acceleration mechanism, but recent data from the NASA Van Allen Probes [7] has clarified that local acceleration by plasma waves is the main driver. Where and how these waves are generated globally at any given time is still an open space physics question due to the wide range of scales and the nonlinear coupling between them.

The research objectives of this project were to implement essential currently-missing capabilities and obtain a complete fully-integrated framework that allows to study the SCE dynamics on a global scale, including micro-scale processes. Specifically, SHIELDS had the following overarching technical goals:

- **Goal 1:** Improved Representation of Substorm Dynamics in Global Simulations
- **Goal 2:** Investigation of Plasma Waves and their Feedback on Global Dynamics
- **Goal 3:** Testing, Validation, and Application of the SHIELDS Framework

Scientific Approach and Results

SHIELDS uses numerical models as powerful tools to specify space weather globally and to place sparsely available space measurements into global context. Given the complex multiscale physics in the magnetosphere, analysis and understanding SCE dynamics requires models that are targeted at key regions/physics regimes. However, the coupling of these models across multiple spatial and temporal scales remains an extreme challenge. SHIELDS leverages from the University of Michigan Space Weather Modeling Framework (SWMF, [8]), that integrates interoperating models of physics domains into a high-performance coupled model. Major SHIELDS developments (Figure 1) are the addition to the SWMF of new kinetic models - iPIC3D [9] and RAM-SCB [10] and data assimilation tools [11]. Such additions provide crucial coupling to microphysics responsible for the SCE, thereby obtaining an improved specification of magnetic reconnection, substorm injections, and plasma wave dynamics. The models are coupled together by the framework code including a control module that determines the overall time-stepping and communication between the models. The

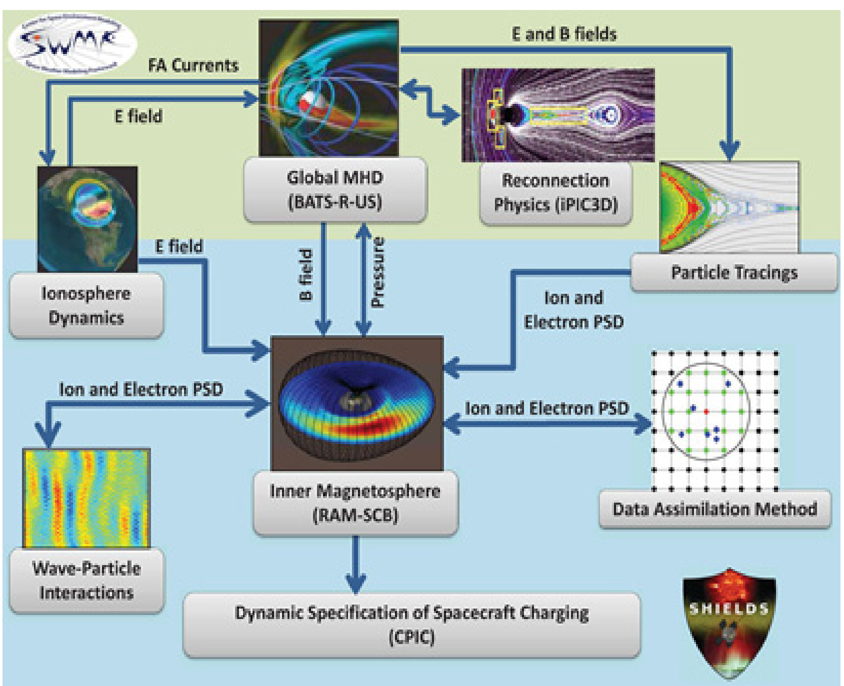

Figure 1. *SHIELDS flow chart showing how this software connects macro- and micro-scale models and combines the results with data-assimilation tools to capture the severity of the spacecraft charging environment. Adapted from [12].*

control module also determines when the coupling among models should occur, the order in which it happens, and it takes care of grid interpolation and synchronization of the model runs to allow for a physically meaningful coupling. Figure 1 shows a flow chart of how the various macro- and micro-scale models used in SHIELDS are inter-connected and how the information is exchanged among them; all couplings among the regional models have now been completed. Further advancements on the three major SHIELDS goals are presented below.

- **Goal 1:** Improved Representation of Substorm Dynamics in Global Simulations

1.1 Large-Scale Particle Tracing

The injection of hot (keV) particles – the primary source of the SCE – into the inner magnetosphere is enhanced during geomagnetic storms and substorms. An important step for the successful modeling of geomagnetic storm dynamics is the two-way coupling of global Magnetohydrodynamic (MHD) models which provide a realistic global solution with "drift codes" that represent well the plasma dynamics in the inner magnetosphere, which is dominated by drift physics whereby particles of different energies, charges, and species move differently from one another. This differential drift motion radically complicates the dynamics near the Earth – in exactly the regions that are most susceptible to spacecraft charging effects.

In the SHIELDS project, the global magnetosphere is modeled with the Block Adaptive Tree Solar wind Roe-type Upwind Scheme (BATS-R-US) [13, 14] MHD code developed at the University of Michigan. MHD codes can model the three-dimensional (3D) magnetosphere with reasonably fine grid resolution faster than real time on a small cluster (to simulate 1 day of magnetospheric activity requires less than a day in computational time). BATS-R-US is driven by solar wind data applied as upstream boundary conditions while the other boundaries let the plasma flow out of the domain. The inner boundary conditions are provided by the Ridley Ionosphere Model (RIM) [15] driven by field aligned currents (FAC) from BATS-R-US. As discussed above, the inner magnetosphere has more complicated physics than what an MHD code can capture, therefore we have coupled BATS-R-US and RIM with the large-scale kinetic code of the inner magnetosphere developed at Los Alamos, the Ring current-Atmosphere interactions Model with Self-Consistent magnetic (B) field (RAM-SCB) [10].

The coupling of the RAM-SCB code to the rest of the SHIELDS framework was a non-trivial task, which is now accomplished. Full two-way coupling of RAM-SCB with the global MHD model has been implemented for single fluid, multi-species, and full multi-fluid approaches as well as MHD with anisotropic ion pressure. Electric potential values are mapped from the RIM ionosphere to be used by RAM. Magnetic field coupling from MHD to the SCB solver is also done through the framework. Simulations using the expanded coupling features show significant advancement in reproducing geomagnetic storm dynamics with a stronger ring current and in better agreement with observations [16, 17]. Nevertheless, one of the last major outstanding dynamical processes in the magnetosphere – substorms – occurring on a timescale of minutes could still not be well-represented, and the Particle Tracing Model (PTM) [18, 19] was developed to solve this problem for the first time in a global space weather model.

The PTM in SHIELDS is a large-scale particle tracing code designed to specify the outer boundary conditions needed by the inner magnetosphere RAM-SCB code with substorm energetic particle dynamics included. To accomplish this, we implemented a "backwards

Liouville test-kinetic" particle tracing approach [18]. The particles are started at the points of interest (e.g., points along the RAM-SCB outer boundary), and then traced backwards in time through the dynamic electric and magnetic fields from the global simulation. We stop each particle far enough in space and time that all of the energization is captured in the final results. The method relies on Liouville's theorem which states that the so-called Phase Space Density (PSD) is conserved on a dynamical trajectory through "phase space". This method allows for the obtained PSD in the tail to be converted to particle fluxes at the original point of the RAM-SCB outer boundary.

Our PTM implementation in SHIELDS traces particles (relativistically) using two different strategies: (1) full orbit integration which follows the full gyro-motion of a particle as it gyrates, bounces and drifts, and (2) guiding center integration which follows only the center-of-gyration of a particle (bounce and drift only.) The full orbit method is simple but computationally expensive and susceptible to build-up of numerical errors, while the guiding-center approach involves more complex equations of motion, it is much faster, but is also not valid where magnetic field gradients are too large. Based on local conditions, the SHIELDS-PTM code is able to dynamically switch between full-orbit and guiding-center tracing in order to optimize results. When switching from guiding-center to full orbit equations of motion, a random gyro-phase is selected to continue. Since such switching introduces an element of stochasticity to the final flux determinations, we average the results over a distribution of initial gyro-phases in order to minimize bias and reduce noise. The SHIELDS-PTM code is fully parallel and designed to work efficiently on high performance computers like LANL's Grizzly and Wolf machines.

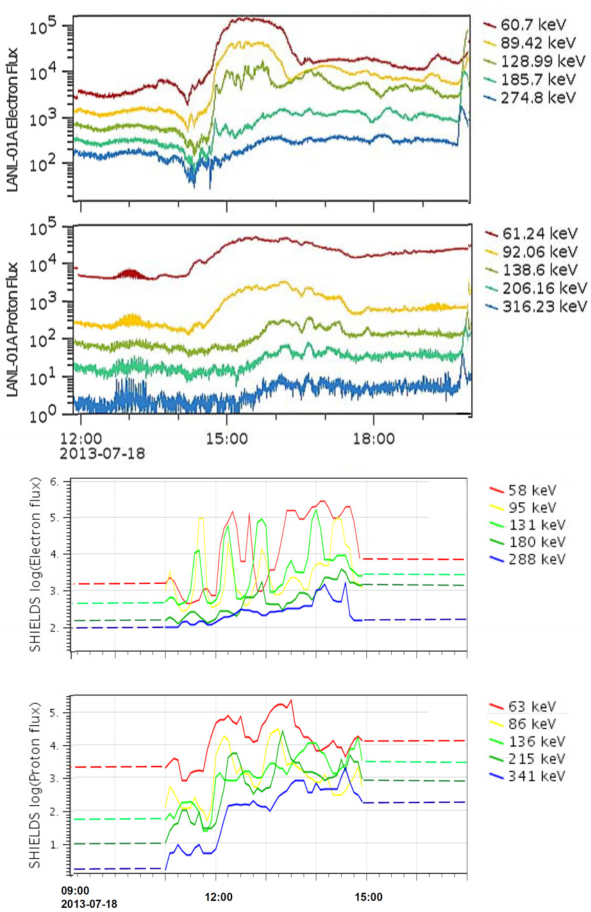

Figure 2. *Simulation of a substorm injection using the SHIELDS-PTM code. The simulated fluxes are normalized to the initial conditions. The overall general characteristics are qualitatively reproduced. Adapted from [12].*

Initial tests of the SHIELDS-PTM code were made on an idealized substorm interval generated in the coupled framework by using interplanetary magnetic field (IMF) input conditions that ramped down to strong negative values for several hours. A substorm consisting of a global reconfiguration of the magnetotail (near-Earth reconnection on the night side and release of a plasmoid down tail) was generated and provided the time varying substorm disturbance fields. The SHIELDS-PTM code was able to generate an energetic particle flux enhancement similar to what is typically observed.

Following this initial test, SHIELDS-PTM was run on realistic substorm intervals in order to compare with actual observations [19, 12]. Figure 2 shows the results for a substorm which occurred on July 18, 2013. The top two panels show energetic electron and proton fluxes from the LANL Geosynchronous SOPA instruments on the LANL-01A spacecraft. The bottom two panels show the energetic electron and proton fluxes simulated at this spacecraft using the SHIELDS-PTM model. The time scale for both observations and simulation are the same, however they are shifted relative to one another since the simulation did not reproduce the injection time. Note that the timing difference is likely a result of the MHD simulation since it's a challenge for global MHD models to accurately describe when a substorm is going to occur based only on solar wind inputs. As explained in section 1.2, we are addressing this challenge by embedding a PIC module in BATS-R-US to allow reconnection physics to develop more realistically in MHD-EPIC and provide a better substorm timing; this will be explored in future work. Of importance to this project is that the overall general characteristics of the injection were qualitatively reproduced. Specifically, it is the first time that a global simulation shows the rapid flux increases of the SCE at lower energies, which are crucial for the forensic analyses.

Finally, to better constrain the specification of the PSD at the location where the particle's backward tracing is stopped, we have implemented a data-optimized model for the PSD sources that can be tuned on an event by event basis [18]. We found that optimized source distributions generally provide a far superior result than statistical models of the source region (as used in the example shown in Figure 2), improving the accuracy of modeled fluxes at some energies by more than an order of magnitude. These innovations, together with the successfully coupled RAM-SCB and PTM codes into the SHIELDS framework provide – for the first time – a realistic specification of the spacecraft charging environment in global simulations.

1.2 Reconnection Physics

As discussed above, a non-trivial challenge for global MHD models, due to the missing microphysics, is that typically they cannot reproduce the fast reconnection rates observed in kinetic simulations. On the other hand, particle-in-cell (PIC) codes have been used with great success in studies of kinetic phenomena like magnetic reconnection. PIC codes solve the full set of Maxwell's equations for the electromagnetic fields, coupled with the equations of motion for electrons and ions. However, they are usually restricted to local simulations due to their high computational cost.

To address this challenge and improve the accuracy of substorm phenomenology in SHIELDS, the BATS-R-US code [14] was two-way coupled with a regional PIC code [9], thus obtaining an exceptional capability, the MHD with Embedded PIC (MHD-EPIC) algorithm [20, 21]. The PIC code covers the regions where kinetic effects are important while the rest of the domain is handled by the fluid code. The implicit particle-in-cell code iPIC3D [9] was integrated into the SWMF as the first model representing the new Particle-in-Cell (PC) component. A general parallel coupler was implemented since the existing SWMF couplers were not suitable for passing the large amount of data between the two massively parallel models. The new coupler keeps the grid description and interpolation methods private for the models. This eliminates the need to describe the grid in an abstract manner and to pass this information to the SWMF or the coupled model. The coupling is very efficient and takes less than 2% of the execution time in all simulations. The coupling between BATS-R-US and iPIC3D works in 3D, and the two grids do not need to be aligned. In addition, multiple PIC regions may be used. This new efficient and flexible coupler was used to model Ganymede's magnetosphere in 3D with 4 PIC regions. The results gave excellent agreement with Galileo measurements, much better than with Hall MHD, showing that the MHD-EPIC algorithm provides a better description of reconnection than the fluid models [21].

Most recently we have applied MHD-EPIC to the Earth [22], which is the main target for the SHIELDS project. This is a very challenging problem, because the ion inertial length, the spatial scale magnetic reconnection originates at, is very small compared to the system size. In this initial application, we have put the PIC box around the dayside reconnection site, as it is smaller than the tail reconnection. Even this is very expensive unless we artificially increase the kinetic scales by changing the ion mass per charge of particles. To check the effect of ion mass per charge on the global solution, we performed a series of 2D MHD-EPIC simulations for an Earth-like system [23]. We found that the results are insensitive, suggesting that we can increase the ion mass per charge and still obtain physically correct solutions on the resolved scales. Using this idea, we performed 3D MHD-EPIC simulations [22] with an ion mass per charge set to 16. The simulation worked very robustly and efficiently. We thus simulated an hour of real time with constant solar wind driving with negative IMF B_Z and found several flux ropes forming at the dayside reconnection site covered by the PIC region. Figure 3 shows some highlights from this MHD-EPIC simulation [12]. The dayside magnetopause is covered by a PIC box, which is represented by the red box in the left panel. Magnetic reconnection happens inside the PIC box and generates flux transfer events (FTEs). The right panel shows a 3D view of three FTEs. Several global and small scale phenomena that are properly reproduced by the simulation are described in [22], including virtual satellite observation of FTEs, signatures of the lower hybrid drift instability (LHDI), and the crescent shape velocity distribution functions observed by the MMS spacecraft.

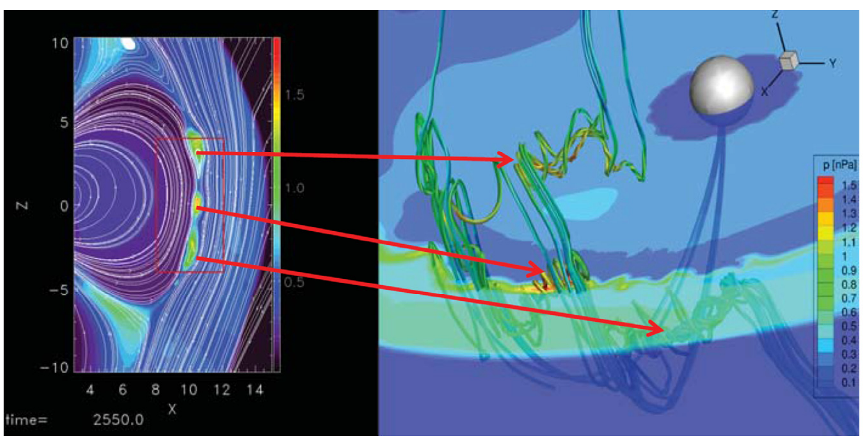

Figure 3. *The FTEs from MHD-EPIC simulation of the Earth's magnetosphere. The left panel shows the pressure (nPa) and the projected magnetic field lines at the meridional plane. The red box represents the region covered by the PIC code. The right panel is the 3D view at the same time. The plasma pressure at the z = 0 plane, and the FTEs colored by pressure are shown. Demonstrates that MHD-EPIC is an efficient approach to kinetic modeling in a global system. Adapted from [12].*

Thanks to the MHD-EPIC algorithm and the increased ion mass per charge we could perform this global simulation with a relatively small and coarse PIC grid while still properly capturing the kinetic reconnection process. This simulation required only 2000 core hours per minute, about 65,000 times faster than what it would take to run with the proton mass per charge ratio and another factor of 10,000 faster than what it would take to run with a global PIC model. We have already performed some preliminary simulations with the MHD-EPIC model where the PIC region covers the Earth's tail reconnection. This allows us to study the substorm process with a kinetic reconnection model for the first time.

1.3 Data Assimilation

We have built a data assimilation scheme [11] to improve the specification of the SCE in SHIELDS. Our approach uses data from near-Earth orbiting satellites to correct for input errors (e.g., in the initial and boundary conditions) which eventually result in inaccuracies in the physics-based RAM-SCB model results. The assimilation procedure can correct for these errors and/or missing physics processes within the model. Data assimilation has proven to be a robust method for reconstructing the radiation belt environment [e.g., 24, 25, 26], but there have only been a few attempts to apply the approach to the ring current environment [27, 28].

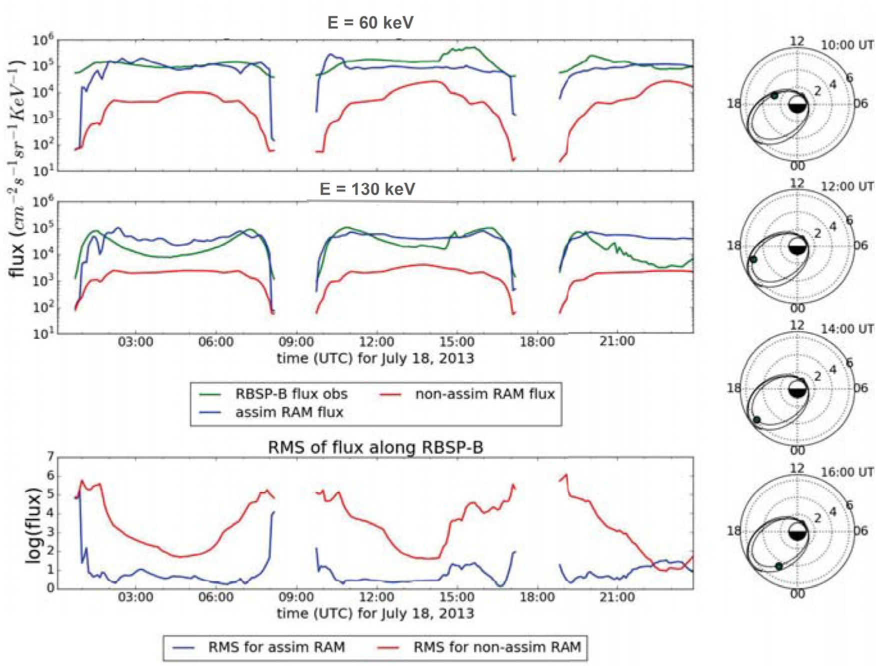

Figure 4. *(top) Spin-averaged flux spectrogram for observations from RBSP-B (green line), assimilated RAM-SCB results using RBSP-A observations (blue line), and unassimilated RAM-SCB (red line). (bottom) Root-mean-square error of the flux along the RBSP-B satellite showing that the data assimilation is moving the model state much closer to the observations. The right plots show the trajectory of the Van Allen Probe B. Adapted from [11].*

Our approach is a variant of the ensemble Kalman filter (EnKF) [29, 30]. We modify the basic method by performing the assimilation on an orthonormal projection of the RAM-SCB state space that captures the dominant modes of variation within the model. This projection, which is similar to principal component analysis or empirical orthogonal functions, helps prevent the data from pushing the model state into unstable regions. To ensure robustness, we also apply an adaptive inflation technique [31] as well as a localization approach of [32].

Further, we have also developed a prototype for a new variant of the ensemble Kalman filter that uses ideas from sparse matrix estimation [33]. The goal of this approach is to regularize the ensemble covariance estimation which can be difficult since the ensemble size is usually much smaller than the size of the state space. This approach could potentially take the place of or reduce the need for localization because it can automatically determine the important conditional dependence relationships in the large state space.

We implemented our data assimilation method to the RAM-SCB model for a substorm event on July 18, 2013 using the Van Allen Probes flux data [11]. We corrected the state of the ring current using proton flux data from Van Allen Probe A and compared the assimilated results with data from Van Allen Probe B. The results showed that the assimilation provided a dramatic improvement of the RAM-SCB model results by nudging the model flux closer to the derived flux from the Van Allen Probes (Figure 4). Over the bulk of the experiment time interval simulated, our assimilation approach reduced the error in flux by at least an order of magnitude and often several orders of magnitude. These results show that data assimilation is a promising approach for improving estimates of the SCE. Subsequently, as part of the GEM/CCMC Spacecraft Charging Challenge, we are investigating a large storm that occurred on March 17, 2013. This data set includes both proton and electron fluxes from the Van Allen Probes A and B. The combination of both data sources into the data assimilation into RAM-SCB provides an improved ring current state than the assimilation with only protons (previous work). The preliminary results look very encouraging, showing several injections of particles propagating inwards of the domain, as observed by both probes. We are finalizing a paper where these results will be presented.

- **Goal 2:** Investigation of Plasma Waves and their Feedback on Global Dynamics

Storms/substorms drive plasma waves that redistribute energy throughout the collisionless magnetospheric environment and couple low-energy plasma with high-energy particles. We explored several aspects of adding the effects of these waves on the large scale dynamics of the SCE as discussed below.

2.1 Validity of the Quasi-Linear Theory of Wave-Particle Interactions

Quasi-linear theory is a framework for modeling the interaction of plasma waves and charged particles. We provided a new assessment of the validity of this theory in the inner magnetosphere. Quasi-linear theory predicts diffusive behavior, in pitch angle and energy, for electrons traversing regions where plasma waves exist. A number of studies [34, 35] have questioned whether this theory is correct at large wave amplitudes where the random “jumps” in electron pitch angle and energy are large. To resolve this issue, we introduced and applied a new methodology to this problem. Rather than search for linear-in-time diffusive behavior in test particle simulations, we solved the Fokker-Planck (FP) equation – with appropriate boundary conditions – and compared the FP-equation predicted electron distribution with the simulated test particle distributions. Our main results showed that (1) quasi-linear theory is valid for a much greater range of wave energies than previously considered, and (2) boundary-condition effects can obscure a linear-in-time region for the growth in particle variance, however this obscurity does not invalid quasi-linear theory [36]. These results provided the necessary justification for using the quasi-linear diffusion framework in RAM-SCB.

2.2 Global Transport and Quasi-Linear Diffusion in RAM-SCB

We investigated the combined effects from time-dependent transport and scattering by whistler-mode waves on the SCE using our RAM-SCB model [10, 37]. This model solves the bounce-averaged kinetic equation for the hot (keV) ion and electron populations in the inner magnetosphere, taking into account all key source and loss processes. The magnetic field is calculated self-consistently with the anisotropic ring current plasma pressure and used subsequently to propagate the particle distributions. We coupled RAM-SCB with a new time-dependent plasmaspheric electron density model based on [38] since one of the key parameters controlling wave-particle interactions (WPI) is the ratio of the electron plasma frequency to the electron gyro frequency. The plasmaspheric densities can decrease sharply by as much as a factor of ten during a geomagnetic storm as the plasmapause is pushed inwards. We investigated the electron precipitation to the atmosphere and found it in good agreement with NOAA/POES and DMSP measurements [39]. RAM-SCB simulations including both pitch angle and energy scattering based on quasi-linear theory, showed that the modeled electron flux at low energies was in good agreement with observations. The simulations showed the initial formation of an asymmetric ring current that evolved into a more symmetric one with storm development. However, the local acceleration by plasma waves of freshly injected electrons was unexpectedly large and led to an overestimation of the fluxes observed with Van Allen Probes (Figure 5). We discovered that this acceleration by WPI occurring at the sharp injection boundary may extend down to energies as low as ~50 keV and could affect significantly the SCE [40]. This high-impact publication was also part of a Los Alamos Science Highlight.

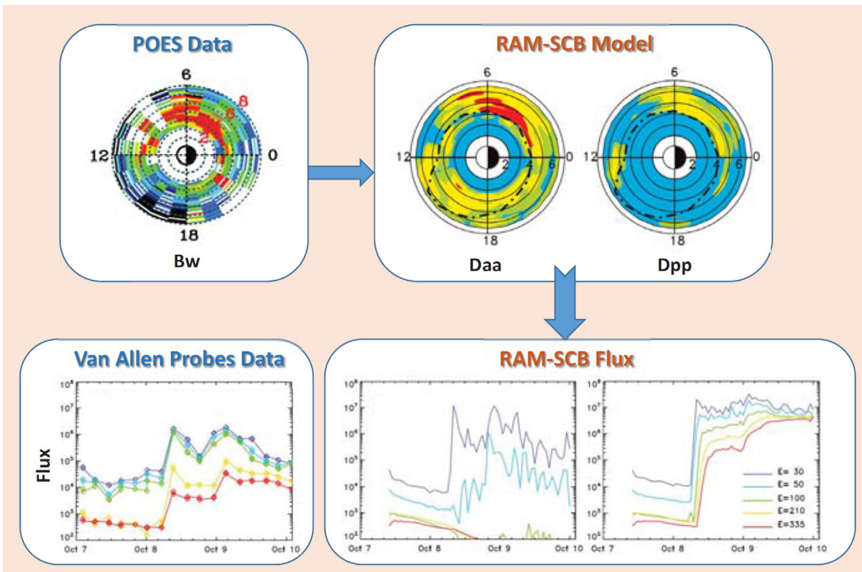

Figure 5. *(top) Schematic representation of RAM-SCB model driven by plasma wave models from POES and Van Allen Probes data. (bottom) Comparison of Van Allen Probes flux data (left) with RAM-SCB simulations without (middle) and with (right) local acceleration by plasma waves. The significant electron acceleration by plasma waves seen in RAM-SCB simulations at energies as low as ~50 keV was not expected. Adapted from [40].*

2.3 Off-Line PIC Simulations and RAM-SCB Diffusion Coefficients

One of the most challenging tasks of the SHIELDS project was to improve the representation of WPI in RAM-SCB via the self-consistent coupling with off-line PIC simulations. A fundamental limitation of the representation of WPI in global models is the assumed spatio-temporal distribution of plasma waves from global climatologies that have been generated over several decades from satellite measurements. These data therefore represent an average state of the magnetosphere and are not event specific. The more sophisticated climatologies are Kp-dependent, but even these may still not be representative of the true wave fields for any given storm [39]. In principle, the anisotropic electron distributions simulated by RAM-SCB predict whether waves could be produced at every point and at all times in its domain. In practice, utilization of this information is confounded by a massive separation of scales: the microscopic coupling of wave and electrons occurs locally, over a scale of a few kilometers, while the inner magnetosphere encompasses a quadrillion cubed km. As a first step in utilizing the electron velocity distribution predicted by RAM-SCB to inform WPI, we have performed PIC simulations for environmental conditions at a select number of points where the predicted distribution anisotropy which drives the waves is large [41]. We found that whistler-mode waves were excited and grew exponentially, propagating mainly along the background magnetic field. The high anisotropy of hot (10's keV) electrons distinctly dropped when the waves were fully developed, and these whistler-mode waves were subsequently damped by the cooler (few keV) electron population. Our simulations verified that the waves generated from RAM-SCB's most anisotropic electron distributions are broadly consistent with the largest wave-amplitudes that are observed during storms. Moreover, the locations and times of these predicted, most unstable distributions are very consistent with satellite observations. These results indicate that off-line PIC simulations could be used to inform WPI in RAM-SCB. Further work in this direction is ongoing.

- **Goal 3:** Testing, Validation, and Application of the SHIELDS Framework

3.1 Configuration and Testing

The computational complexity of the multi-scale, multi-physics problem that SHIELDS is solving requires the integration of multiple distinct physics and numerical packages into a single coherent framework. This project successfully incorporated all SHIELDS components into a single version control system. Using Git Submodules the SHIELDS project combined components together in a single repository, while allowing each component to be developed individually. Component integrations tests were performed in an automated fashion using Gitlab continuous integration (CI) infrastructure that the SHIELDS project helped prototype, implement and fund.

The SHIELDS framework is designed to run at large scale on the world's most powerful supercomputers. For such advanced applications, the SHIELDS software can be built from source following the instructions detailed in the user manual (visit SHIELDS public website: http://www.lanl.gov/projects/shields/ for details). However, a critical part of the SHIELDS design philosophy is to allow both users and developers to get working with SHIELDS on any system without having to deal with complicated software dependencies. As such, the SHIELDS framework has been packaged in a Docker image, allowing installation and deployment with a single command on any laptop, desktop, or high-performance computing system with Docker installed.

To facilitate the release of the SHIELDS application through Docker we developed an automated continuous deployment (CD) pipeline as shown in Figure 6. The SHIELDS application is kept automatically up to date with the latest SHIELDS developments. As changes are made to the

SHIELDS code-base, they are automatically built and tested using Travis Continuous Integration. If all tests pass, a new Docker image is built reflecting the code changes and pushed to DockerHub. SHIELDS framework releases are automatically tagged with the corresponding change to the source code. Finally, to streamline the setup process and to reduce input errors, we have developed an Easy-to-use Graphical Interface for SHIELDS (AEGIS). This tool allows users to select their components of interest, set relevant parameters, and generate various input files and execution scripts needed to achieve a desired modeling result.

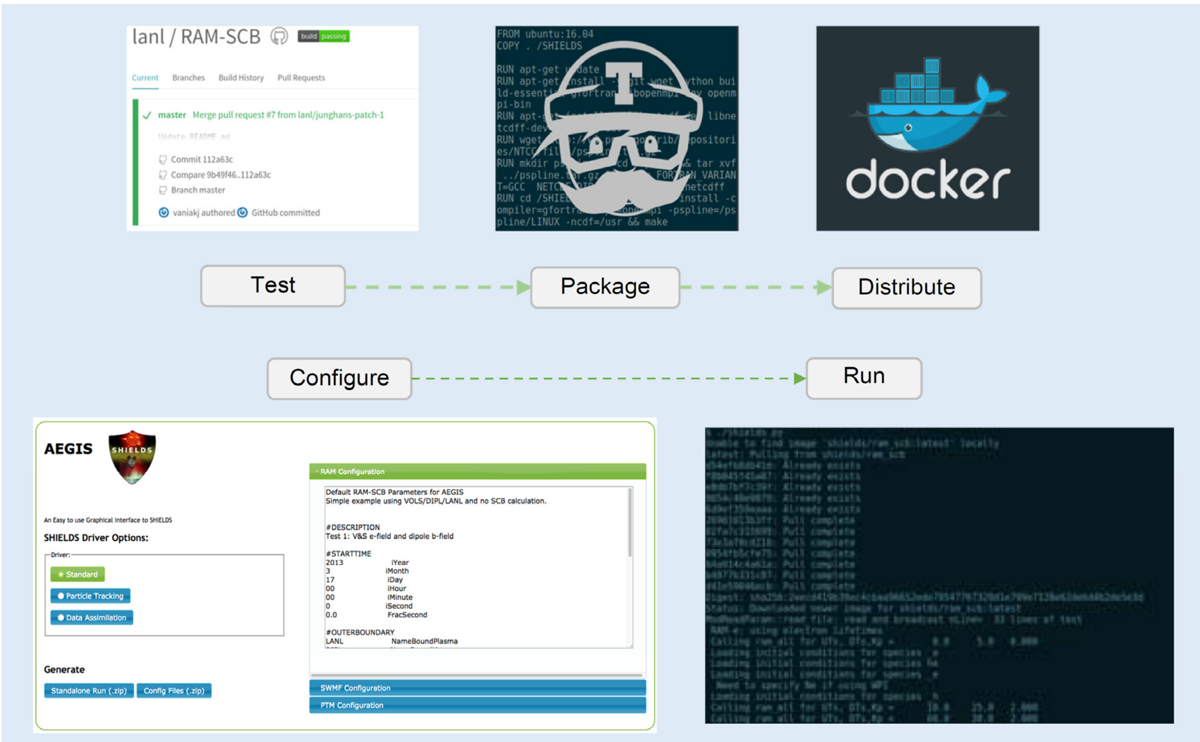

__Figure 6.__ This figure demonstrates the automated workflow behind the compilation, testing and deployment of SHIELDS. By packaging of SHIELDS with Docker and AEGIS we enable rapid deployment and execution of SHIELDS on local machines, traditional clusters and cloud infrastructure.

3.2 Spacecraft Surface Charging

A unique feature of the SHIELDS framework is the possibility to calculate the surface charging of a spacecraft with any geometry by means of an electrostatic Particle-In-Cell (PIC) code known as Curvilinear PIC (CPIC) [42, 43]. Problems involving the interaction of complex material objects with plasmas are challenging computationally because of their multiscale nature: the characteristic spatial (and possibly temporal) scales of the object must be resolved in the simulation in addition to the characteristic scales of the plasma, thus making the problem 'more multi-scale' and requiring additional sophistication compared to standard PIC methods. For instance, at geosynchronous orbit the characteristic scales of the plasma like the electron Debye length or the electron gyro-radius are hundreds of meters while the spacecraft characteristic size is on the order of meters, with features that could be even smaller. For these reasons, most tools developed for spacecraft charging calculations [44, 45, 42, 43] use non-uniform, adaptive meshes which conform to the surface of the spacecraft.

A critical aspect in the design of spacecraft-charging codes is the choice of the computational mesh. Several approaches use unstructured meshes, i.e. meshes where cells carry no predefined ordering, and where a connectivity map is necessary to locate cell neighbors. Unstructured meshes give enormous flexibility for the generation of computational domain conforming to extremely complex objects and have become the method of choice in the computational fluid dynamics community. Unfortunately, their computational performance in the context of PIC codes is seriously degraded by issues associated with data locality and indirect data access patterns. In order to avoid these issues, CPIC is based on multi-block structured meshes [43]. These meshes are structured (i.e. have a predefined connectivity pattern that makes localization of cell neighbors trivial) at the level of the individual blocks but unstructured in a global sense and present new challenges, such as discontinuities in the mesh properties and mesh orientation changes across adjacent blocks. These challenges have been met by a new approach [43] that uses: (1) a curvilinear formulation of the PIC method; (2) a mimetic finite-difference discretization of Poisson's equation suitable to address the challenges of multi-block meshes; (3) a hybrid (logical-space position/physical-space velocity coordinates), asynchronous particle mover. As a result, geometric accuracy associated with curvilinear, multi-block meshes is complemented by the significant performance and computational efficiency associated with the aforementioned field solver and particle mover. In addition, CPIC is highly parallelized and runs efficiently on thousands of processors.

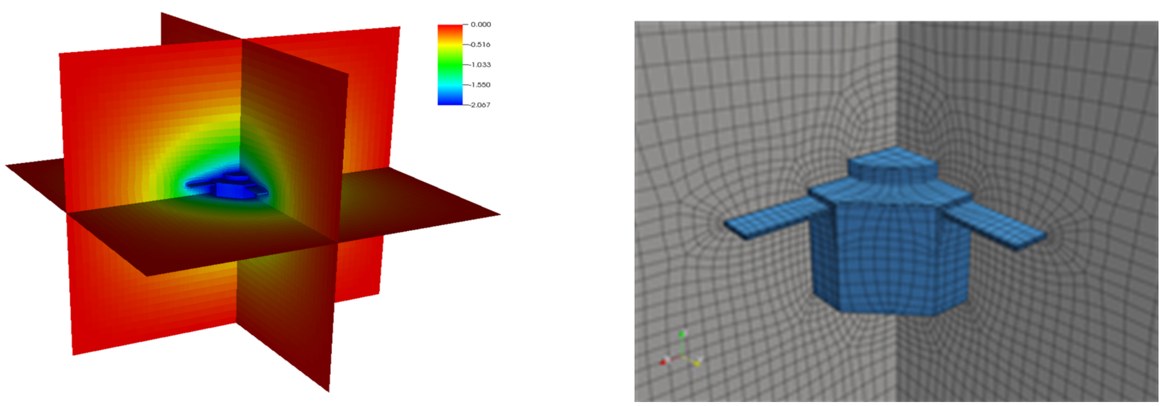

Figure 7. *On the left, the electrostatic potential (normalized to 5 eV) around the Van Allen Probes spacecraft arising from the cold plasma distribution obtained by SHIELDS on March 17th 2013 at UT=10, L=5 and MLT=6. On the right, part of the curvilinear multi-block mesh conforming to the surface of the Van Allen Probes spacecraft. CPIC provides the connection between occurrence of anomalies and SCE dynamics.*

CPIC has been successfully interfaced to the SHIELDS framework, thus meeting one of the goals of the LDRD project. SHIELDS outputs the plasma environment around the spacecraft, which typically consists of two plasma populations whose relative densities and temperatures are critical in determining the level of surface charging of the spacecraft. The first is the cold plasma, characterized by temperatures of a few eV, and represented in CPIC by a Maxwellian distribution function. The warm plasma, with temperatures of the order of keV, is loaded in

CPIC with the appropriate distribution (often non-Maxwellian). Given the geometry of the spacecraft and its material properties, and the characterization of the plasma environment by SHIELDS, CPIC computes the level of surface charging via the local electric field and particle fluxes around the spacecraft. An illustrative example of this calculation is shown in Figure 7, where the cold plasma population produced by SHIELDS for the March 17th 2013 storm (at 10 UT, L drift shell of 5 and magnetic local time of 6) was used to calculate the spacecraft charging of a geometry representative of the Van Allen Probes spacecraft. In this example the spacecraft charges to about -10 V. A paper comparing the spacecraft-charging prediction from SHIELDS with actual Van Allen Probes data is in preparation as part of the Spacecraft Charging Challenge we are organizing in collaboration with NSF/GEM and CCMC.

Anticipated Impact on Mission

The SHIELDS framework is a new space weather capability that improves our understating of magnetosphere dynamics and positions LANL at the forefront of space science exploration. Its reanalysis and forecast capabilities enhance the Laboratory's national security mission to understand, assess, and predict natural and man-made threats to the space infrastructure. The SHIELDS framework will motivate strategic partnerships in the area of growth of "space weather" and lead to new funding opportunities: (1) to reanalyze past events (of interest to satellite operators, Aerospace, DOD); (2) to uncover new magnetospheric physics and causal relations between events (NASA, NSF, DOD); (3) to perform now-casting and forecasting (NSWP, DOD, NASA, NSF). We will continue the interactions with the Feynman Center for Innovation on promoting SHIELDS and to connect with industrial companies which could be interested in SHIELDS. The initiatives we have been involved so far are listed below.

I. We are exploring practical applications of the SHIELDS framework to analyze surface charging events on the GPS MEO satellites. These satellites lack plasma measurements in the energy ranges expected to correlate with surface-charging events. We are discussing potential sources of funding with the GPS program to correlate anomalies with the surface charging environment predictions by SHIELDS.

II. SHIELDS (and its capabilities for magnetic field line mapping and spacecraft charging) provides critical simulation support for both the design and interpretation of the CONNEX project, a mission concept to use compact relativistic electron guns fired from a spacecraft to trace magnetic field lines from the magnetosphere to the ionosphere. We plan to propose the CONNEX mission to the NASA Middle Explorer Call that is anticipated in FY18.

III. A high priority recommendation of the 2013 Solar and Space Physics Decadal Survey is the implementation of DRIVE-Inspired Integrative Science Centers to tackle key space science problems that require multidisciplinary teams of theorists, observers, modelers, and computer scientists. We have submitted a response to NASA's RFI in August 2017 and plan to propose a DRIVE-Inspired Integrative Science Center to be hosted at LANL once the solicitation is released in the 2018 timeframe.

IV. A significant impact of the SHIELDS project is the role it played in moving forward software engineering practices and technologies at LANL. SHIELDS had an active role in the development and deployment of LANL's gitlab.lanl.gov continuous integration (CI) infrastructure. gitlab.lanl.gov is actively used by over 600 LANL employees and hosts nearly 1000 projects, many of which rely on dedicated CI infrastructure.

V. Because of its optimal algorithmic design choices, CPIC is a unique tool for plasma-material interaction problems. Although at present no direct accuracy/performance comparison against other spacecraft-charging codes exists, our preliminary estimates indicate that CPIC should be at least a factor of 5-10 faster than a corresponding PIC code on unstructured meshes [43]. Considering that some spacecraft-charging codes are not parallelized, the performance gain can easily become several orders of magnitude. For these reasons, CPIC can solve a broader set of plasma-material interaction problems, some of which are outside the scope of SHIELDS. Examples of the successful application of CPIC include ongoing efforts to study the feasibility of emitting a high-power electron beam from a magnetospheric spacecraft [46, 47] and the interaction of dust particles with magnetic fusion energy plasmas [48].

VI. Hazardous conditions in the inner magnetosphere, known as "space weather" can damage or disable civilian and military space assets. Acknowledging that space weather is a global challenge, the White House OSTP released the National Space Weather Action Plan, followed by an Executive Order in October 2016, to develop a response and recovery plan. Important components of this plan include developing predictive models and transitioning space-weather models from research to operations. We are thus developing a near real-time version of the SHIELDS framework (Figure 8) that allows for the prediction of the inner magnetosphere plasma environment using RAM-SCB. An option exists to output spacecraft-charging environment spectra and plot them along given satellite trajectory. This mode is best suited for long term simulations with operational implications (e.g. monitoring Dst, satellite-specific charging environments, etc.). In this mode, the external boundary conditions are provided by newly-developed models [49, 50], capable of predicting electron and ion fluxes at GEO with about an hour of lead time using upstream solar wind data and several hours of lead time using a prediction of Kp to drive the model. We expect that this capability will promote strategic partnerships with government or commercial customers (DOE, DOD, NOAA, FAA, satellite operators, etc.); currently, two companies have expressed interest. It may also be appropriate for inclusion into

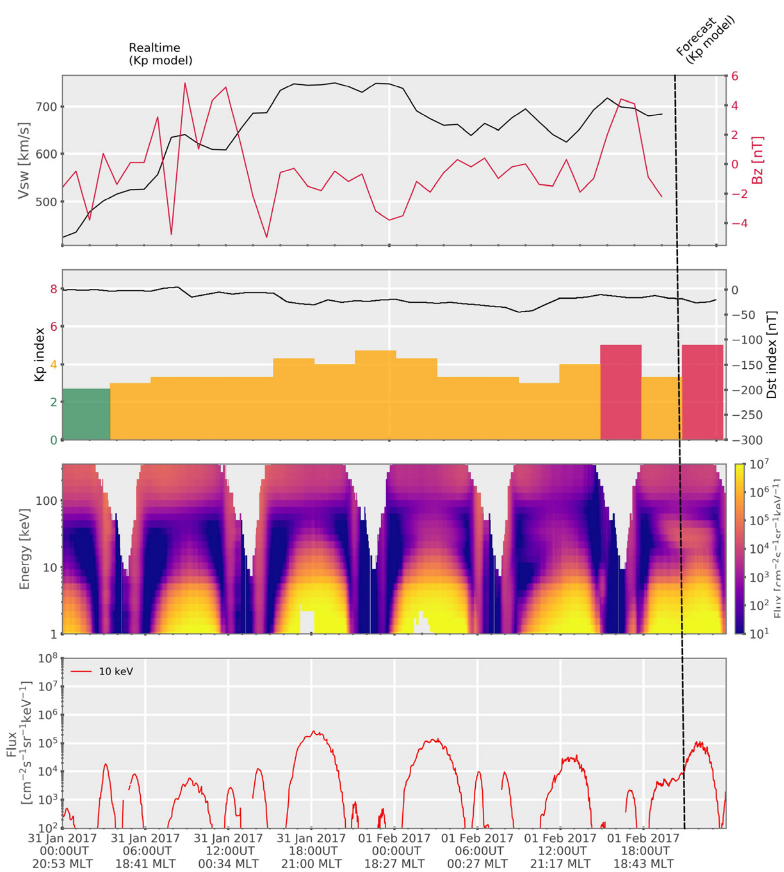

Figure 8. *Output of the SHIELDS near real-time model showing a 3 hour prediction along Van Allen Probe-A satellite trajectory.*

programmatic modeling frameworks of the space environment like DIORAMA.

VII. We organized several workshops sponsored by CNLS and CSES to foster awareness about space weather hazards and their mitigation. The SHIELDS workshop "Shielding Society from Space Weather" held in 2016 in Santa Fe was a big success with large number of participants and a press release in PCmag and a LANL Science Highlight. In addition, we initiated a Spacecraft Charging Challenge at the NSF/GEM workshop as part of the benchmark challenges that are used by NASA Community Coordinated Modeling Center (CCMC) to evaluate Geospace environment models.

VIII. The SHIELDS framework is one of the Lab's eight innovations that were selected as finalists for the 2017 R&D 100 Awards. These prestigious awards honor the top 100 technological advances of the past year. This highlights SHIELDS success in technical innovation for national security science. A YouTube video showcasing the SHIELDS Space Weather Platform to the public is on display at the Bradbury Science Museum in Los Alamos.

Conclusion

The spacecraft surface charging environment (SCE) is one of the main space weather hazards that occur in the most heavily satellite-populated region of the Earth's magnetosphere. To forecast SCE and assist spacecraft design and hazard mitigation, we have developed SHIELDS, a new software platform designed to understand, model, and predict the near-Earth space environment; as shown in Figure 1, at the end of the 3-year LDRD project all couplings among the regional models in SHIELDS have been accomplished. Using a multi-disciplinary team and state-of-the-art models and computational facilities, we investigated important physics questions related to particle injection and acceleration associated with magnetospheric storms and substorms, as well as plasma waves. Major highlights from the SHIELDS project are:

1) SHIELDS is the first software platform to successfully couple a global MHD (BATS-R-US) with a particle-in-cell (iPIC3D) code for the Earth's magnetosphere; this coupling represents the most efficient approach to resolving magnetic reconnection physics and substorm dynamics in a global system.
2) SHIELDS achieves the first data assimilation for the inner-magnetosphere model (RAM-SCB), demonstrating an order of magnitude improvement in the accuracy in the simulation of the spacecraft surface charging environment.
3) SHIELDS provides a more self-consistent treatment of global transport and scattering by plasma waves. This feature helped unravel the physics of cross-energy coupling in the Earth's radiation belts. It showed for the first time that acceleration of freshly injected electrons by plasma waves may be significant at energies that affect the SCE.
4) SHIELDS unique calculations of spacecraft surface charging can evaluate the hazards of SCE for specific satellites/spacecraft geometry and their relation to the near-Earth space environment.

The SHIELDS framework is an end-to-end model of the magnetosphere driven by the dynamic solar wind that enhances our capability to reliably model and predict the near-Earth space environment where operational satellites reside. To follow major accomplishments of the project, including those from future development, please visit SHIELDS public website: http://www.lanl.gov/projects/shields/.

References

1. Baker, D. N., L. J. Lanzerotti, Resource Letter SW1: Space Weather, *Am. J. Phys*., **84**, p. 166, doi:10.1119/1.4938403 (2016).
2. Fennell, J. F., H. C. Koons, J. L. Roeder, and J. B. Blake, Spacecraft charging: Observations and relationship to satellite anomalies, *ESA Special Publications SP-476,* 279 (2001).
3. Thomsen, M. F., M. G. Henderson, and V. K. Jordanova, "Statistical properties of the surface-charging environment at geosynchronous orbit", *Space Weather*, **11**, p. 237, doi:10.1002/swe.20049 (2013).
4. Burch, J. L., "The fury of space storms"*, Sci. American*, **284**, p. 86, doi:10.1038/scientificamerican0401-86 (2001).
5. Baker, D. N., et al., Severe space weather events–understanding societal and economic impacts workshop report. Technical Report ISBN: 0-309-12770-X, National Research Council (2008).
6. Van Allen, J. A., G. H. Ludwig, E. C. Ray, C. E. McIlwain, "Observation of high intensity radiation by satellites 1958 Alpha and Gamma", *Jet Propulsion*, **28**, 9, pp. 588, doi: 10.2514/8.7396 (1958).
7. Reeves, G. D., H. E. Spence, M. G. Henderson, et al., "Electron acceleration in the heart of the Van Allen radiation belts", *Science*, **341**, 991, doi: 10.1126/science.1237743 (2013).
8. Toth, G., et al., Space Weather Modeling Framework: A new tool for the space science community, *J. Geophys. Res*. **110** (A12), doi:10.1029/2005JA011126 (2005).
9. Markidis S., G. Lapenta, Rizwan-uddin, "Multi-scale simulations of plasma with iPIC3D", *Mathematics and Computers in Simulation*, **80** (7), 1509-1519 (2010).
10. Jordanova, V. K., S. Zaharia, and D. T. Welling, "Comparative study of ring current development using empirical, dipolar, and self-consistent magnetic field simulations", *J. Geophys. Res*., **115**, A00J11, doi:10.1029/2010JA015671 (2010).
11. Godinez, H. C., Y. Yu, E. Lawrence, M. G. Henderson, B. Larsen, V. K. Jordanova, Ring current pressure estimation with RAM-SCB using data assimilation and Van Allen Probe flux data, *Geophys. Res. Lett.* **43**, doi:10.1002/2016GL071646 (2016).
12. Jordanova, V. K., et al., Specification of the near-Earth space environment with SHIELDS, *J. Atm. Sol.-Terr. Phys*., under review (2017).
13. Powell, K. G., P. L. Roe, T. J. Linde, T. I. Gombosi, and D. L. De Zeeuw, "A solution-adaptive upwind scheme for ideal magnetohydrodynamics", *J. Comp. Phys*., **154**, 284–309 (1999).
14. Toth, G., B. van der Holst, I. V. Sokolov, D. L. De Zeeuw, T. I. Gombosi, et al., "Adaptive Numerical Algorithms in Space Weather Modeling", *J. Comp. Phys*., **231**, 870, doi:10.1016/j.jcp.2011.02.006 (2012).
15. Ridley, A., T. Gombosi, D. Dezeeuw, "Ionospheric control of the magnetosphere: conductance", *Ann. Geophys.,* **22**, 567-584 (2004).
16. Welling, D. T., V. K. Jordanova, A. Glocer, G. Toth, M. Liemohn, and D. Weimer (2015), The two-way relationship between ionospheric outflow and the ring current, *J. Geophys. Res. Space Physics*, **120**, 4338–4353. doi: 10.1002/2015JA021231.
17. Welling, D. T., G. Toth, V. K. Jordanova, Y. Yu, Integration of RAM-SCB into the Space Weather Modeling Framework, *J. Atm. Sol.-Terr. Phys*, under review (2017).
18. Woodroffe, J., T. V. Brito, V. K. Jordanova, M. G. Henderson, S. K. Morley, M. H. Denton, Data-optimized source modeling with the Backwards Lioville Test-Kinetic method, *J. Atm. Sol-Terr. Phys*., doi:10.1016/j.jastp.2017.09.010 (2017).
19. Brito, T. V., J. Woodroffe, V. K. Jordanova, M. Henderson, J. Birn, Particle tracing modeling of ion fluxes at geosynchronous orbit, *J. Atm. Sol.-Terr. Phys*., under review 2017.

20. Daldorff, L., G. Toth, T. I. Gombosi, G. Lapenta, J. Amaya, S. Markidis, J. U. Brackbill, "Two-way coupling of a global Hall magnetohydrodynamics model with a local implicit Particle-in-Cell model", *J. Comput. Phys.*, **268**, 236, doi:10.1016/j.jcp.2014.03.009 (2014).
21. Tóth, G., X. Jia, S. Markidis, B. Peng, Y. Chen, L. Daldorff, V. Tenishev, D. Borovikov, J. Haiducek, T. Gombosi, A. Glocer, J. Dorelli, Extended magnetohydrodynamics with Embedded Particle-in-Cell simulation of Ganymede's magnetosphere, *J. Geophys. Res*. **121**, doi:10.1002/2015JA021997 (2016).
22. Chen, Y., G. Tóth, P. Cassak, X. Jia, T. I. Gombosi, J. A. Slavin, S. Markidis, I. B. Peng, V. K. Jordanova, M. G. Henderson, Global three-dimensional simulation of Earth's dayside reconnection using a two-way coupled magnetohydrodynamics with embedded particle-in-cell model: initial results, *J. Geophys. Res*., doi:10.1002/2017JA024186 (2017).
23. Tóth, G., Y. Chen, T. I. Gombosi, P. Cassak, S. Markidis, and I. B. Peng, Scaling the ion inertial length and its implications for modeling reconnection in global simulations, *J. Geophys. Res*., doi:10.1002/2017JA024189 (2017).
24. Bourdarie, S., R. H. W. Friedel, J. Fennell, S. Kanekal, T. E. Cayton, Radiation belt representation of the energetic electron environment: Model and data synthesis using the Salammb radiation belt transport code and Los Alamos geosynchronous and GPS energetic particle data, *Space Weather* **3** S04S01. doi:10.1029/2004SW000065 (2005).
25. Shprits, Y., D. Kondrashov, Y. Chen, R. Thorne, M. Ghil, R. Friedel, and G. Reeves, Reanalysis of relativistic radiation belt electron fluxes using CRRES satellite data, a radial diffusion model, and a Kalman filter, *J. Geophys. Res. (Space Physics),* **112**, A12216, doi:10.1029/2007JA012579 (2007).
26. Godinez, H. C., J. Koller, Localized adaptive inflation in ensemble data assimilation for a radiation belt model, *Space Weather* **10** S08001. doi:10.1029/2012SW000767 (2012).
27. Garner, T. W., R. A. Wolf, R. W. Spiro, First attempt at assimilating data to constrain a magnetospheric model, *J. Geophys. Res*. **104** 25,14525, 152 (1999).
28. S. Nakano, G. Ueno, Y. Ebihara, M.-C. Fok, S. Ohtani, P. C. Brandt, D. G. Mitchell, K. Keika, T. Higuchi, A method for estimating the ring current structure and the electric potential distribution using energetic neutral atom data assimilation, *J. Geophys. Res*. **113** A05208, doi:10.1029/2006JA011853 (2008).
29. Evensen, G., "Sequential data assimilation with a nonlinear quasi-geostrophic model using Monte Carlo methods to forecast error statistics", *J. Geophys. Res.*, **99**, 10,143–10,162 (1994).
30. Evensen, G., "The ensemble Kalman filter: Theoretical formulation and practical implementation", *Ocean Dyn.*, **53**, 343–367 (2003).
31. Li, H., E. Kalnay, T. Miyoshi, Simultaneous estimation of covariance inflation and observation errors within an ensemble Kalman filter, *Q. J. R. Meteorol. Soc*. **135** 523533 (2009).
32. Hamill, T. M., J. S. Whitaker, C. Snyder, "Distance-Dependent Filtering of Background Error Covariance Estimates in an Ensemble Kalman Filter", *Mon. Wea. Rev.*, **129**, 2776–2790 (2001).
33. Hou, E., E. Lawrence, A. Hero, "Penalized Ensemble Kalman Filters for High Dimensional Non-linear Systems." https://arxiv.org/abs/1610.00195 (2016).
34. Tao, X., J. Bortnik, J. M. Albert, K. Liu, and R. M. Thorne, Comparison of quasilinear diffusion coefficients for parallel propagating whistler mode waves with test particle simulations*, Geophys. Res. Lett*., **38**, L06105, doi:10.1029/2011GL046787 (2011).
35. Liu, K., D. Winske, S. P. Gary, and G. D. Reeves, Relativistic electron scattering by large amplitude electromagnetic ion cyclotron waves: The role of phase bunching and trapping, *J. Geophys. Res*., **117**, A06218, doi:10.1029/2011JA017476 (2012).
36. Delzanno, G. L., C. A. Jeffery, and V. K. Jordanova, Toward a Self-Consistent Treatment of Radiation Belt Wave-Particle Interactions, 32nd URSI General Assembly, Montreal, Canada, 19-26 Aug., 2017.
37. Jordanova, V. K., D. T. Welling, S. G. Zaharia, L. Chen, R. M. Thorne, Modeling ring current ion and electron dynamics and plasma instabilities during a high-speed stream driven storm, *J. Geophys. Res*., **117**, A00L08, doi:10.1029/2011JA017433 (2012).

38. Rasmussen, C. E., S. M. Guiter, and S. G. Thomas, Two-dimensional model of the plasmasphere: refilling time constants, *Planet. Space Sci*., **41**, 35, (1993).

39. Yu, Y., V. K. Jordanova, A. J. Ridley, J. M. Albert, R. B. Horne, C. A. Jeffery, A New Ionospheric Electron Precipitation Module Coupled with RAM-SCB within the Geospace General Circulation Model, *J, Geophys. Res*., **121**, DOI: 10.1002/2016JA022585 (2016).

40. Jordanova, V. K., W. Tu, Y. Chen, S. K. Morley, A.-D. Panaitescu, G. D. Reeves, and C. A. Kletzing, RAM-SCB simulations of electron transport and plasma wave scattering during the October 2012 "double-dip" storm, *J. Geophys. Res. Space Physics*, **121**, doi:10.1002/2016JA022470 (2016).

41. Yu, Y., G. L. Delzanno, V. K. Jordanova, I. B. Peng, S. Markidis, PIC simulations of wave-particle interactions with an initial electron velocity distribution from a kinetic ring current model, *J. Atm. Sol.-Terr. Phys*., to appear in 2017.

42. Delzanno, G. L., E. Camporeale, J. D. Moulton, J. E. Borovsky, E. A. MacDonald, M. F. Thomsen, CPIC: a curvilinear particle-in-cell code for plasma–material interaction studies*, IEEE Trans. Plas. Sci*. **41**, 3577 (2013).

43. Meierbachtol, C. S., D. Svyatsky, G. L. Delzanno, L. J. Vernon, J. D. Moulton, An Electrostatic Particle-In-Cell Code on Multi-block Structured Meshes, to appear in *J. Comput. Phys*. (2017).

44. Mandell, M. J., V. A. Davis, D. L. Cooke, A. T. Wheelock, C. J. Roth, Nascap-2k spacecraft charging code overview, *IEEE Transactions on Plasma Science,* **34,** 2084 (2006).

45. Roussel, J. F., F. Rogier, G. Dufour, J. C.Mateo-Velez, J. Forest, A. Hilgers, D. Rodgers, L. Girard, D. Payan, Spis open-source code: Methods, capabilities, achievements, and prospects, *IEEE Transactions on Plasma Science,* **36,** 2360 (2008).

46. Delzanno, G. L., J. E. Borovsky, M. F. Thomsen, J. D. Moulton, and E. A. MacDonald. Future beam experiments in the magnetosphere with plasma contactors: How do we get the charge off the spacecraft? *J. Geophys. Res. Space Physics,* **120**(5):3647-3664, doi:10.1029/2014JA020608 (2015).

47. Delzanno, G. L., J. E. Borovsky, M. F. Thomsen, and J. D. Moulton. Future beam experiments in the magnetosphere with plasma contactors: The electron collection and ion emission routes, *J. Geophys. Res. Space Physics*, 120, 3588–3602. doi: 10.1002/2014JA020683 (2015).

48. Delzanno, G. L., and Xian-Zhu Tang. Charging and heat collection by a positively charged dust grain in a plasma. *Phys. Rev. Lett.,* **113**:035002, Jul 2014.

49. Denton, M. H., M. F. Thomsen, V. K. Jordanova, M. G. Henderson, J. E. Borovsky, J. S. Denton, D. Pitchford, and D. P. Hartley, An empirical model of electron and ion fluxes derived from observations at geosynchronous orbit, *Space Weather*, **13**, 233-249, doi:10.1002/2015SW001168 (2015).

50. Denton, M. H., M. G. Henderson, V. K. Jordanova, M. F. Thomsen, J. E. Borovsky, J. Woodroffe, D. P. Hartley, and D. Pitchford, An improved empirical model of electron and ion fluxes at geosynchronous orbit based on upstream solar wind conditions, *Space Weather*, **14**, doi:10.1002/2016SW001409 (2016).