Final Report for MIT Portugal Program (MPP) Research Seed Fund Project (2023)

Space Weather Modeling: a Coupled Ionosphere-Thermosphere Physics-Based Approach

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1 Research results and accomplishments

The accurate prediction of aerodynamic drag on satellites orbiting in the upper atmosphere is critical to the operational success of modern space technologies, such as satellite-based communication or navigation systems, which have become increasingly popular in the last few years due to the deployment of constellations of satellites in low-Earth orbit. As a result, physics-based models of the ionosphere and thermosphere have emerged as a necessary tool for the prediction of atmospheric outputs under highly variable space weather conditions.

Physics-based models of the Earth's upper atmosphere are typically based on finite difference or finite volume discretizations of the conservation equations of mass, momentum, and energy for several neutral and charged components. However, the large number of grid points needed to resolve the space and time scales present in the solution of these equations, combined with the complexity of the multi-parameter inputs, can make these models computationally expensive.

The goal of this research project has consisted of developing a high-order, physics-based modeling framework for simulating the ionosphere-thermosphere system, specifically designed to predict upper atmospheric dynamics under different space weather conditions. The model has been implemented in the open-source discontinuous Galerkin (DG) code `Exasim` [1], a computational framework for high-performance computing ensuring scalability and portability to a wide range of computer platforms, including GPU-based architectures. `Exasim` features an implicit-in-time approach, employing diagonally implicit Runge Kutta (DIRK) schemes, and a matrix-free approach, optimized for GPU performance.

1.1 Physics-based model

The project has devised an upper atmospheric model describing the conservation of mass, momentum, energy and charge in the ionosphere-thermosphere system, ranging between 100 and 600km of altitude. Multiple neutral and charged species are considered in the model, namely O, O_2, N, N_2, NO, He, and their corresponding positive ions (O^+, O_2^+, N^+, N_2^+, NO^+, He^+), besides electrons. Such model has been formulated in a Cartesian rotating frame of reference employing cube-sphere meshes, such as the one shown in Figure 1, to avoid pole singularities and provide uniform grid spacing.

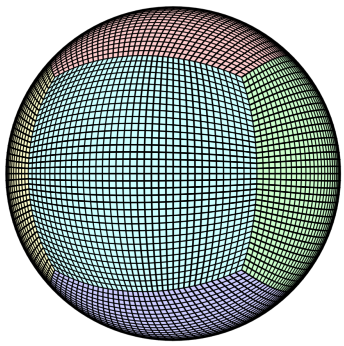

Figure 1: Cube-sphere grid used for simulation.

The conservation equations stem from the compressible Navier Stokes equations and account for chemical reactions, momentum and energy transfer mechanisms, and the effect of the solar activity. The thermosphere employs a non-hydrostatic description in the rotating Earth system. The multiple neutral species are handled considering chemically frozen mass fractions. In this manner, the model specifies variable physical properties with altitude at a reduced computational cost.

A heating source due to extreme ultraviolet radiation accounts for the amount of energy being transferred to the system due to photoionization. This term is responsible for the day-night variability of the upper atmosphere and for its response to solar activity. In addition, photoionization and photoabsorption mechanisms are also responsible for a set of chemical reactions.

The thermospheric model has been extended to account for multiple neutral and charged species (positive ions and electrons). This has required the implementation of a comprehensive chemistry model accounting for nearly 50 reactions of various types. This has allowed increasing the physical fidelity of the model, including as well the effect of collisional processes, multiple energy equations and the effect of electric and magnetic fields. To this end, we have introduced an external description of the magnetic field via an eccentric dipole approximation. In addition, we have prescribed the electric field via an open-closed field line boundary approximation, which defines the high-latitude electric potential as a result of magnetospheric coupling, as shown in Figure 2.

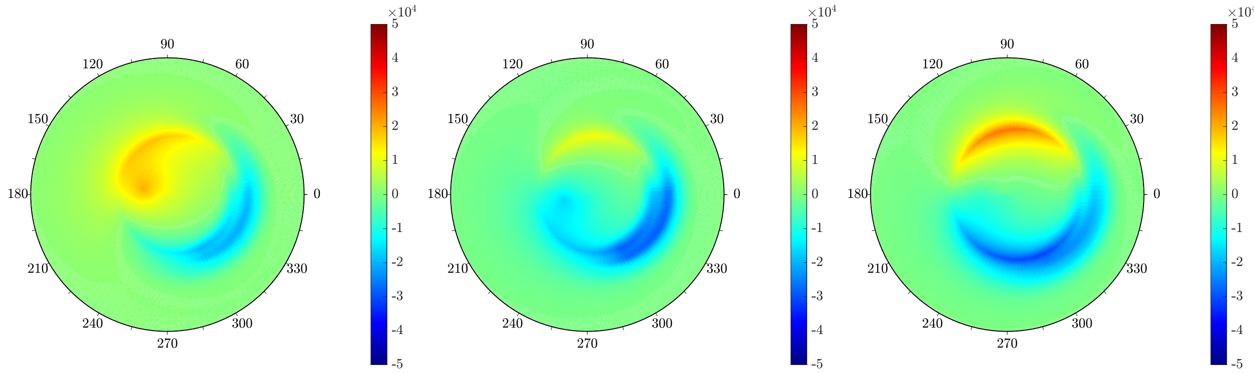

Figure 2: North hemisphere electric potential patterns using an open-closed field line boundary approximation at different instants of time. Representation in magnetic coordinates.

1.2 Model validation and computational studies

Neutral thermosphere study: validation with Swarm A satellite date

The physics-based thermospheric model has been validated by comparing the density estimated derived from the numerical simulations with experimental observations gathered along the Swarm A satellite trajectory [2, 3]. The study was conducted under spring equinox conditions, corresponding to March 20, 2014. During that day, the considered satellite performed approximately 15 orbits around the Earth at an altitude oscillating between 470 and 500km.

The model and experimental results were also compared with predicions obtained from the empirical model MSIS [4] and from the physics-based models GITM [5] and TIE-GCM [6]. The corresponding results are displayed in Figure 3.

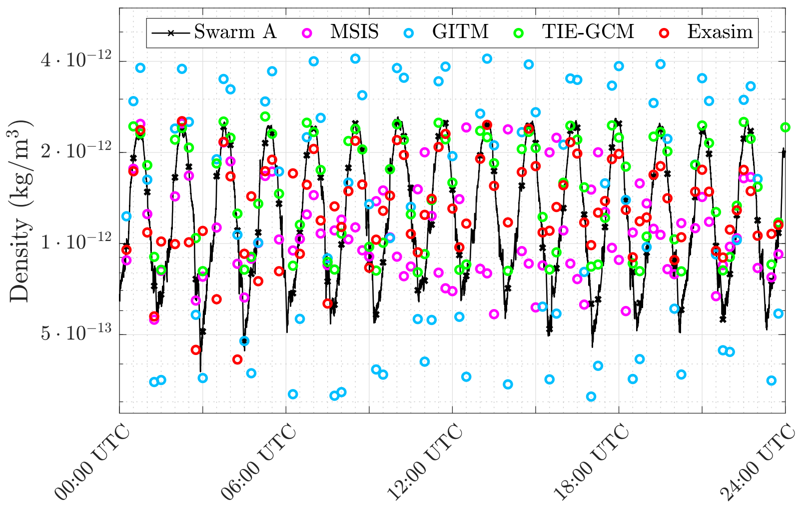

Figure 3: Density predictions of different thermospheric models along the Swarm A satellite trajectory during 20/04/2014, compared to observational data.

The density predictions made by `Exasim` align closely with the satellite estimates, mirroring the behavior of TIE-GCM. Conversely, GITM exhibits larger oscillation amplitudes in this case, leading to both overpredictions and underpredictions of the density along the orbit. Finally, for this case, the empirical model MSIS persistently underestimates the density.

The root mean square error of the different predictions is reported in Table 1 for a quantitative assessment of the accuracy of each approximation. The physics-based ionospheric-thermospheric model TIE-GCM provides the most accurate results, while the proposed physics-based thermospheric model delivers satisfactory density estimates for this case. On the other hand, the predictions from GITM and MSIS display larger degrees of error.

	MSIS	GITM	TIE-GCM	`Exasim`
RMS error	0.5325	0.4871	0.1531	0.2528

Table 1: Root mean square error of the density estimates of different thermospheric models along the Swarm A satellite trajectory with respect to observational data.

This example demonstrates the robust performance of the proposed thermospheric model, providing neutral density predictions along the Swarm A satellite trajectory with error levels comparable to established physics-based models.

Ionosphere-thermosphere tests: chemistry model performance

The ionospheric extension of the model has introduced a set of charged species, with full chemical treatment between neutrals and ions. The chemistry model accounts for nearly 50 reactions of different nature (due to photoionization, photoabsorption, recombination, ion-neutral, neutral-neutral and 3-body reactions).
Initial results have allowed to observe the temporal evolution of different ion species subject to different conditions. An example of this is shown in Figure 4.
The model is solved implicitly and has been implemented within the GPU code. These tests have shown that the resulting time steps are not critically impacted, and are still dominated by the neutral flow dynamics. In addition, the proposed formulation allows for the possibility of ion transport for any of the species.

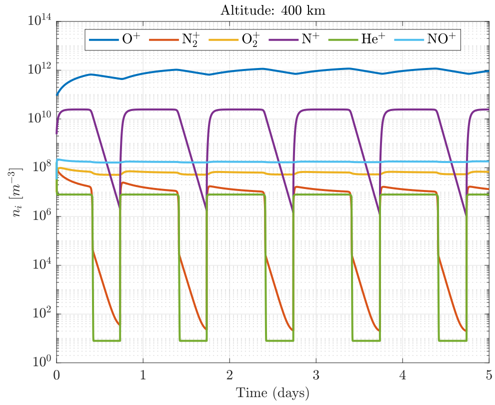

Figure 4: Time evolution of ion number densities at 400km of altitude.

1.3 Further algorithmic developments

Besides the ionospheric model development, additional work has been carried out aimed at improving the computational efficiency of the approach, thus supporting real-time applications and help to advance space weather research To this end, the `Exasim` code has been further developed throughout this project and has incorporated the hybridizable DG (HDG) method [7], together with the existing local DG discretization. The HDG method requires the computation of Jacobians for a matrix-based solution strategy, unlike the previous matrix-free DG approach. This implementation has required the development of an efficient iterative solver for the sparse linear system of equations and the implementation of suitable preconditioners. Such computational development has been aimed at enabling an improved time-marching strategy, with larger time-steps that better accommodate to the problem dynamics.
In addition, `Exasim` has embraced the portability library *Kokkos* for enhanced performance across GPU systems. This strategy has been adopted in order to being able to operate flexibly in different GPU platforms (for instance, from Nvidia GPUs to AMD GPUs).

2 Interactions with our collaborators in Portugal

Initial interactions with our collaborators from Portugal, especially at the beginning of the project, were productive and allowed a deeper understanding of the availability of observational data for ionospheric comparisons and validation. Unfortunately, closing the loop by comparing our computational results with ionospheric experimental data has not happened within the period of grant performance. The development of the ionospheric portion of the model took a significant amount of effort and validation with experimental data has not been performed yet.
The teams were able to have a first meeting in person during the 2023 European Space Weather Week, and our research was also presented in the 2024 edition of the European Space Weather Week, held in Coimbra under the organization of our collaborators.

3 Publications and presentations

The research conducted throughout this project has been disseminated in multiple talks and conferences. In addition, the core of the physics-based model, corresponding to the thermospheric portion of it, had been initially published in [8, 9], although this work had been conducted prior to the start of the MPP 2023 Seed Grant.

Invited Talks

- HAO Colloquium, National Center for Atmospheric Research, Boulder, USA. April 2024.
  J. Vila-Pérez, A computational strategy for physics-based space weather modeling.

- 2024 MIT Portugal Conference, Coimbra, Portugal. November 2024. *(Poster)*
  J. Vila-Pérez, High-fidelity ionosphere-thermosphere modeling: a physics-based discontinuous Galerkin approach

Presentations

- 2024 European Space Weather Week, Coimbra, Portugal. November 2024.
  J. Vila-Pérez, N.C. Nguyen, J. Peraire Towards high-fidelity ionosphere-thermosphere forecasting: a physics-based discontinuous Galerkin approach.
- 2023 AGU Fall Meeting, San Francisco, USA, December 2023.
  J. Vila-Pérez, N.C. Nguyen, J. Peraire An open-source GPU-accelerated discontinuous Galerkin approach for ionospheric and thermospheric modeling.
- 2023 European Space Weather Week, Toulouse, France, November 2023.
  J. Vila-Pérez, N.C. Nguyen, J. Peraire An open-source framework for high-fidelity physics-based space weather modeling on GPU systems: validation and benchmarks.

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