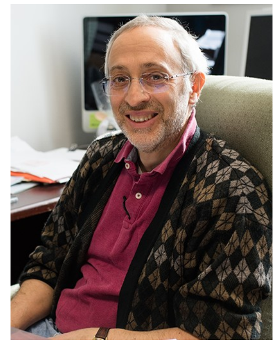
2018-2019 Grand Challenge Award – Final Report



Awardee: **David Goldstein, Professor,**
Aerospace Engineering and Engineering Mechanics

Research Award Title: DSMC Model Development for Earth's Upper Atmosphere

Research Summary

I was the very grateful recipient of a Grand Challenge award during the 2018-2019 academic year. The goals of the effort were to develop a research project to model the Earth's upper atmosphere with the DSMC (direct simulation Monte Carlo) stochastic method. The award allowed me to have teaching relief during the fall of 2018, including time for travel to work with colleagues in Boulder and Ann Arbor, to develop plans for how to link our pre-existing planet-scale DSMC ability to lower atmosphere GCMs.

Review of my GC request: DSMC Model Development for Earth's Upper Atmosphere
Understanding the Earth's weather and climate often involves solving the fluid dynamics equations of motion as a global circulation model or GCM. The difficulties in a GCM in part stem from lack of definite knowledge of the boundary conditions, incomplete understanding of the physics, the broad range of important scales, and the computational resources needed. Above the atmosphere in near-Earth space, the "space weather" environment is becoming increasingly important to understand due to its influence on space operations and communications. In this region, chemistry, radiation and electromagnetic field effects must be accounted for. This is particularly difficult, especially for creating a predictive ability, due to the uncertain forcing of the solar input. Between the continuum atmosphere and space lies a region where thermodynamic, chemical and radiative non-equilibrium occur. This region, extending from the base of the thermosphere up to above the exobase (where the local molecular mean free path begins to exceed the atmospheric scale height), is not modeled well as fully continuum and thus amenable to simulation with some version of the Navier Stokes equations. It is correctly modeled by a version of the Boltzmann equation of rarefied gas dynamics.

Directly solving the Boltzmann equation including the appropriate physical models for chemistry, multiple species, radiation, charged particles, etc. at a planetary scale is infeasible. My group has instead been developing a direct simulation Monte Carlo (DSMC) planet scale simulation ability under NASA sponsorship over many years. In DSMC numerical particles representing molecules, atoms, and ions are moved and collided during a time step. We have applied our code to simulations of plumes and impacts and escape from several moons and small bodies in the solar system and developed within it a broad range of physics modules. I have also recognized that there is a strong scientific argument why our same DSMC methods and codes can now be brought home to Earth. The “grand challenge” in this problem is to provide a predictive ability to simulate upper atmospheric conditions a couple of days into the future, better than is currently possible. I believe we now have the method – DSMC – that correctly links the continuum lower atmosphere models with the magneto-hydrodynamic space models. But scientific/physics models are incomplete and real engineering issues remain. These issues include true unsteady hybridization between the continuum, DSMC and MHD regions, coupling of radiation transport across domains, general inter-code data compatibility, running linked but different codes in parallel, gross inhomogeneity of actual boundary data, etc. Beyond such issues, there exist fundamental science questions we can uniquely address such as: how do upwardly propagating gravity waves spread and break and deposit energy to heat the thermosphere? These open issues were explored as part of the Grand Challenge award.

During the autumn of 2018 I traveled to Boulder to meet with planetary atmosphere colleagues at NCAR (Stan Solomon, National Center for Atmospheric Research), at NOAA (Tim Fuller-Rowell) Dan Scheeres and Steve Nerem, at UCB, Fran Bagenal and Vincent Dols, at LASP (Laboratory for Atmospheric and Space Physics, at UCB) and Leslie Young and John Spencer at SwRI-Boulder. I also gave a presentation at NOAA on DSMC on Earth atmospheric modeling.

A U. Michigan in Ann Arbor, I met with Andrew Nagy, Tamas Gombosi, Mike Liemohn, Aaron Ridley, Valeriy Tenishev and Michael Combi to discuss both planetary rarefied atmospherics and the Earth’s upper atmosphere. I also worked with my postdoc, Jordan Steckloff, on our related projects. Discussions with Ridley went very well and we together developed a new way to mutually validate both DSMC approaches and GCM approaches to representing the flow. In particular, we recognized that we could use coincident simulations with DSMC and the GITTM GCM of Ridley to quantify the errors a continuum approximation makes in its representation of the “transport coefficients” like viscosity or thermal diffusivity. Those coefficients are species-specific and the errors become important at high altitudes when the atomic/molecular mean free paths become large and thermodynamic equilibrium ceases to apply. We together wrote a new proposal to AFOSR (for $940,000) titled “Toward the Development of a Hybrid Kinetic-Continuum (DSMC-GCM) Method to Enable Physics-Based Predictions of Earth’s Upper Atmosphere”. We received excellent reviews, but it appears that our price was too high and the AFOSR resources too low. We continue to pursue the ideas with AF.

Related to the AF proposal, I helped my post-doc Arnaud Mahieux develop a new approach to model vertical propagation of gravity waves. Other researchers have recently shown that such waves depart from thermodynamic equilibrium as they “break” and deposit their energy in the uppermost atmosphere. This is certainly important on Earth, but it is also likely critical to understand in order to relate spacecraft-observed atmospheric density profiles at Mars and Venus to the atmospheric temperatures at those altitudes. With my help, Dr. Mahieux developed and submitted two proposals to NASA to incorporate gravity wave simulation with DSMC into interpretation of recent Mars and Venus data. One proposal has failed (alas) and we are waiting to hear about another.