Extending the Upper Boundary of Atmospheric Models

Sarah Luettgen[1], Eric Sutton[1], Jeffrey Thayer[1]*

[1] Aerospace Engineering Sciences Department, University of Colorado at Boulder

**Corresponding Author: sarah.luettgen@colorado.edu*

I. Background and Objective

Background: As the atmosphere becomes less dense with altitude, collisions between particles become increasingly rare. This change in the length of the average distance particles travel between collisions as compared to the density scale height also changes the equations which we use to describe this region of the atmosphere, forcing a shift from fluid equations to a particle kinetic model.

Problem: Fluid model assumptions break down in the upper atmosphere

- Less frequent collisions require additional terms to be included in the fluid equations
- These modifications become increasingly computationally expensive and complex [3]

Objective: create a unified model of the atmosphere from 32 km altitude through the exosphere.

- Couple a fluid model of the lower atmosphere – TIME-GCM – with a particle model of the upper atmosphere - MONACO
- Ensure both models output the same values in overlapping regions
- Initiate two-way coupling: both simulations exchange information about their current state

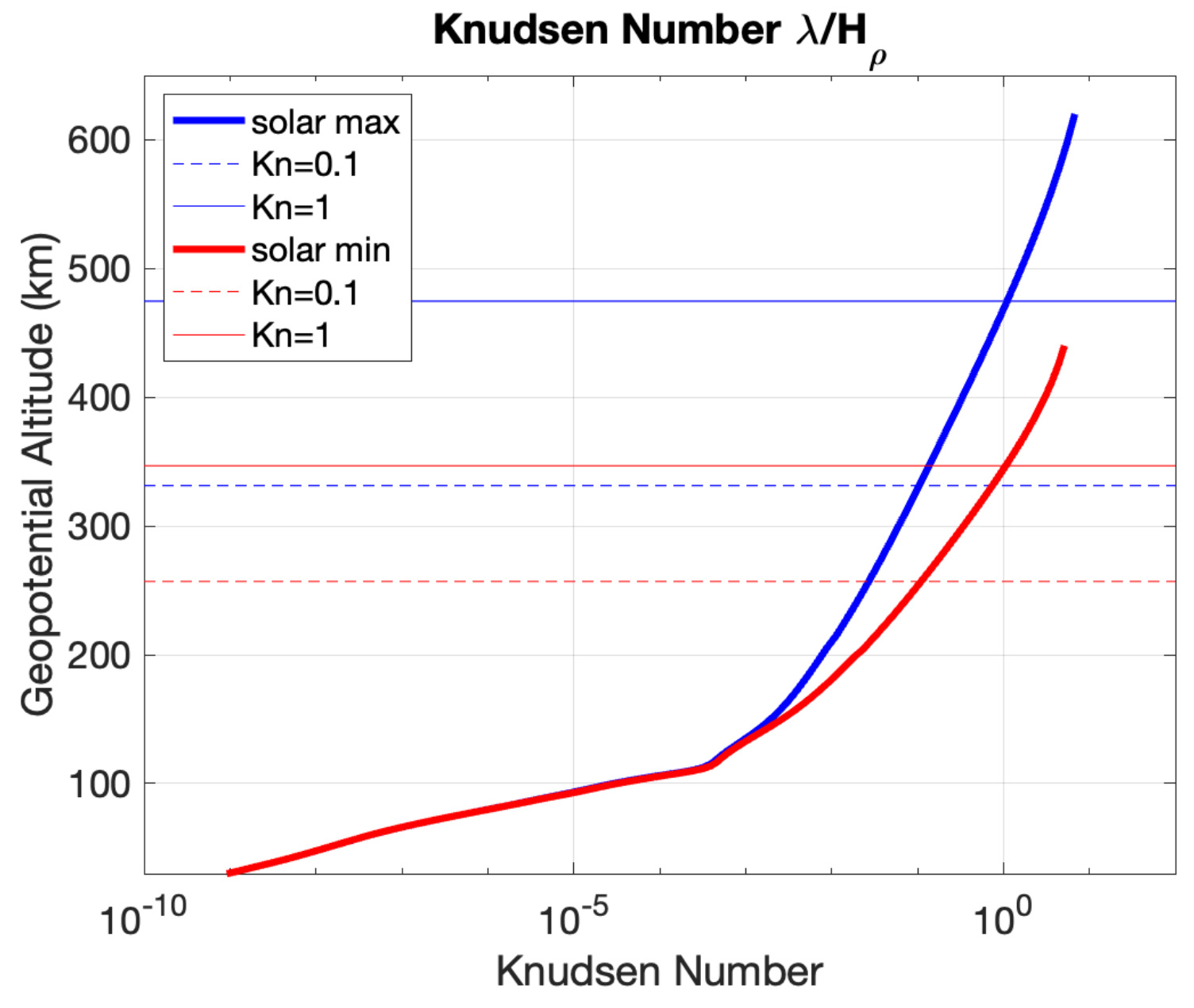
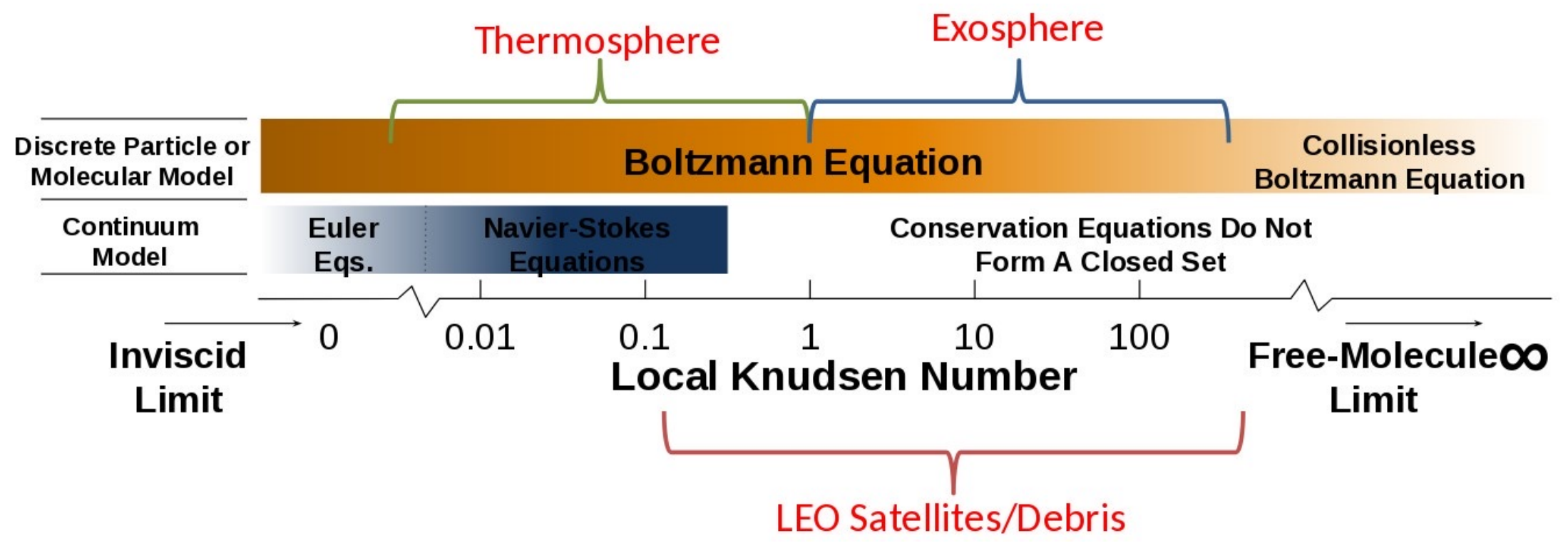


Fig 1. The Knudsen number (Kn), mean free path divided by density scale height, for different solar conditions. The transition region ($0.01 < Kn < 10$), where infrequent collisions disrupt the equilibrium of the gas, encompasses the upper thermosphere through the lower exosphere.

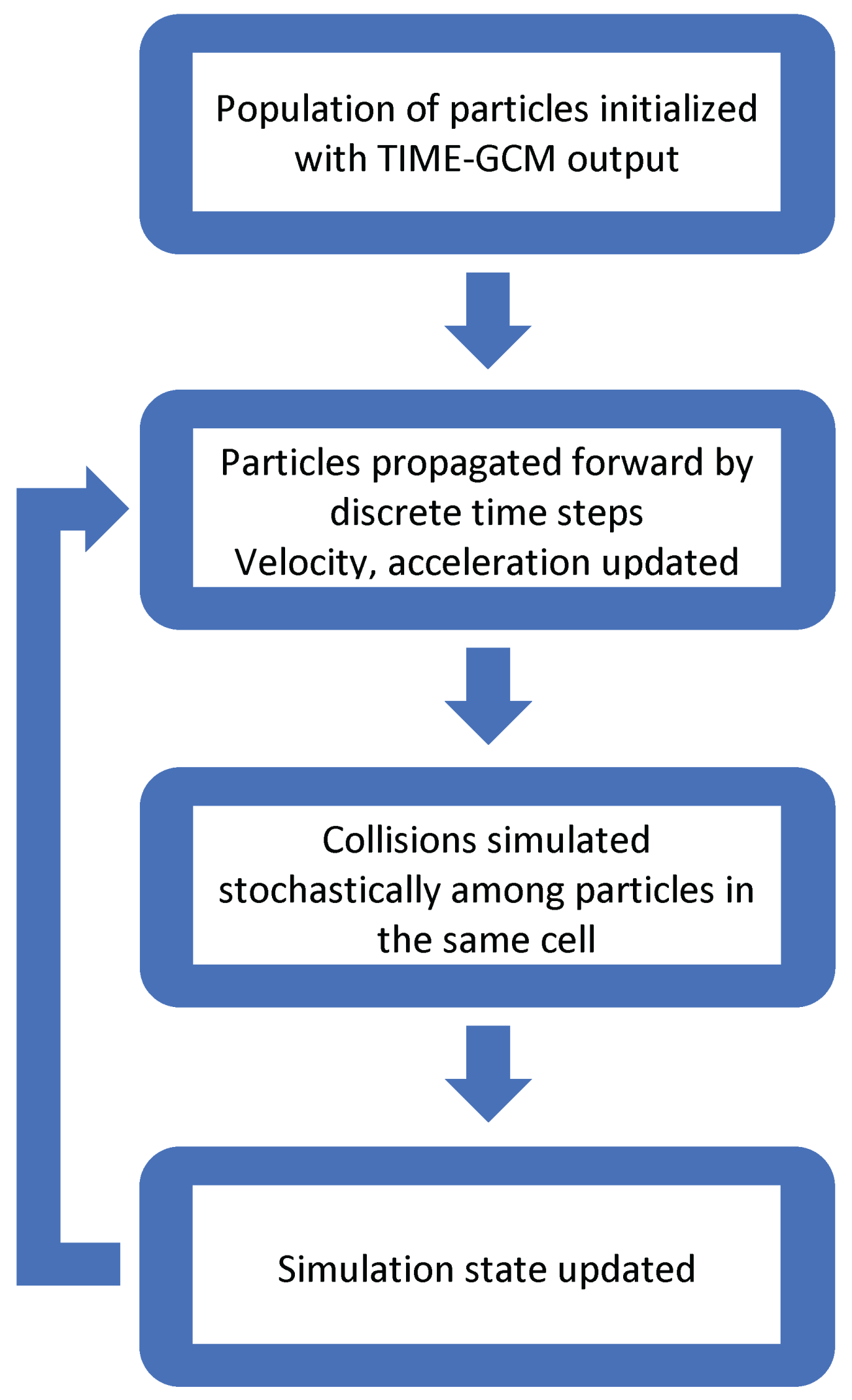


Left: Fig 2. Applicability of equation sets to an atmospheric regime based on Knudsen number. Modified from [1].

II. Significance

- Provide a coupled, physical description of the upper atmosphere and exosphere, significantly extending the upper boundary of TIME-GCM.
- Improve accuracy in projecting drag affecting the orbital trajectories of spacecraft and debris, minimizing spacecraft maneuvers and decreasing the risk of collisions [7].
- Provide a better understanding of atmospheric escape without assuming a Maxwellian distribution of particles and a collisionless exosphere (e.g., [4]).

III. Direct Simulation Monte Carlo (DSMC) Particle Model


Population of particles initialized with TIME-GCM output

Particles propagated forward by discrete time steps
Velocity, acceleration updated

Collisions simulated stochastically among particles in the same cell

Simulation state updated

Fig 3. DSMC algorithm. A grid of cells is formed and populated with particles. The particles are propagated forward in discrete time steps. The process then repeats [2].

Advantage: DSMC models solve the Boltzmann equation while avoiding the high computational expense of direct integration [1]. No need to make assumptions about the velocity distribution of particles [3].

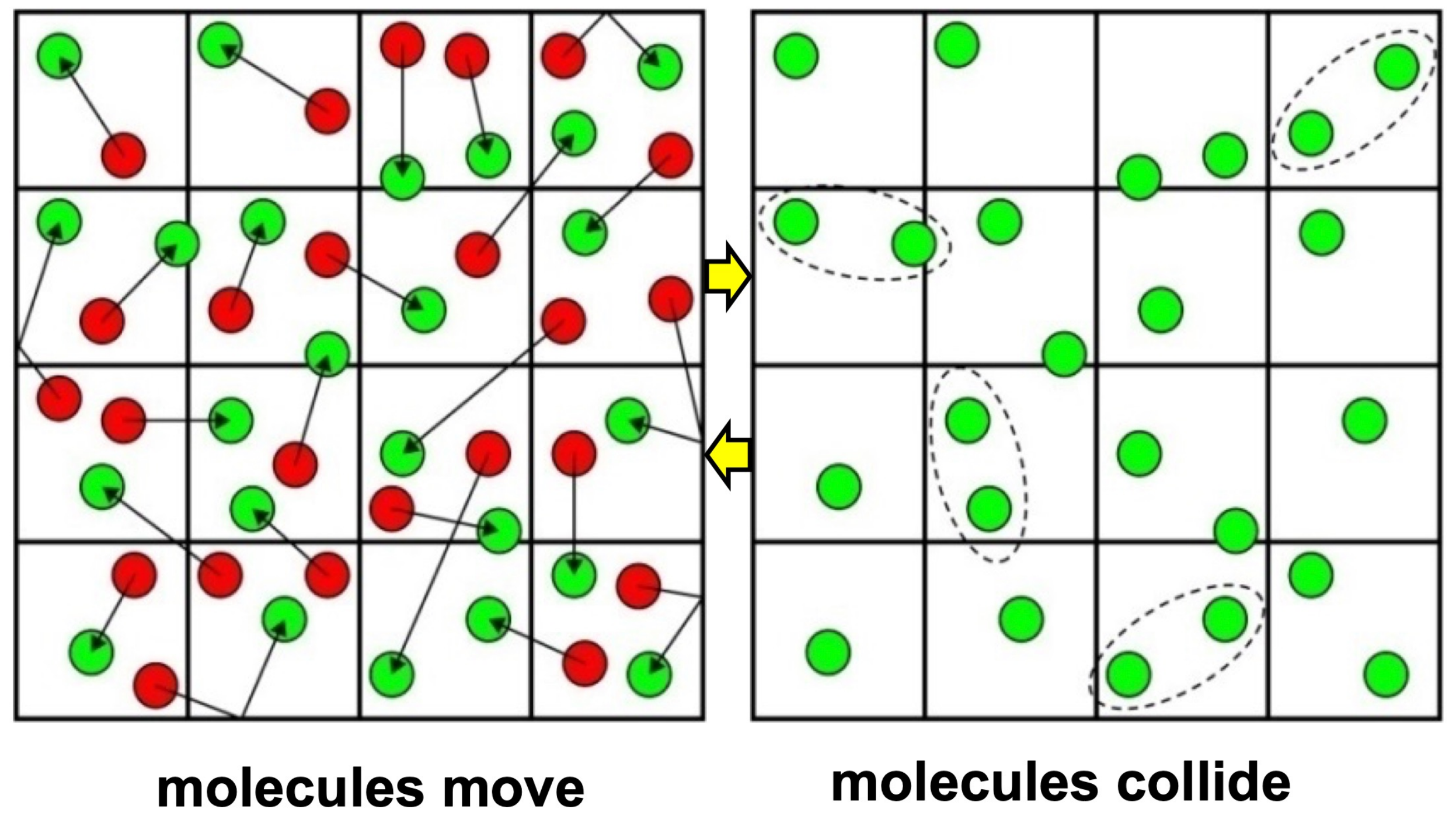


Fig 4. Only particles within the same cell (i.e., within one mean free path) are chosen for collisions. Figure from [5].

Requirements [3]:

- Time step < mean collision time
- Cell dimension < mean free path
- Dilute gas for which the ratio of the interparticle spacing to the particle size is at least ~7
- A small number of simulation particles is used to represent the full number of particles in the atmosphere

IV. DSMC Exospheric Model

Exospheric particle model

- A DSMC algorithm is being adapted to function as a model of the exosphere
- The grid of 3-dimensional cells begins at 362 km and forms 36 spherical layers ("shells") that extend radially outward
- Forces that govern the motion of particles: gravitational, Coriolis, centrifugal, & collisional

Outputs

- Collision rate
- Mean free path
- Mass density
- Number density
- Pressure
- Translational, rotational, & vibrational temperature
- Velocity in x, y, z directions
- Species: O, N2, He, & H

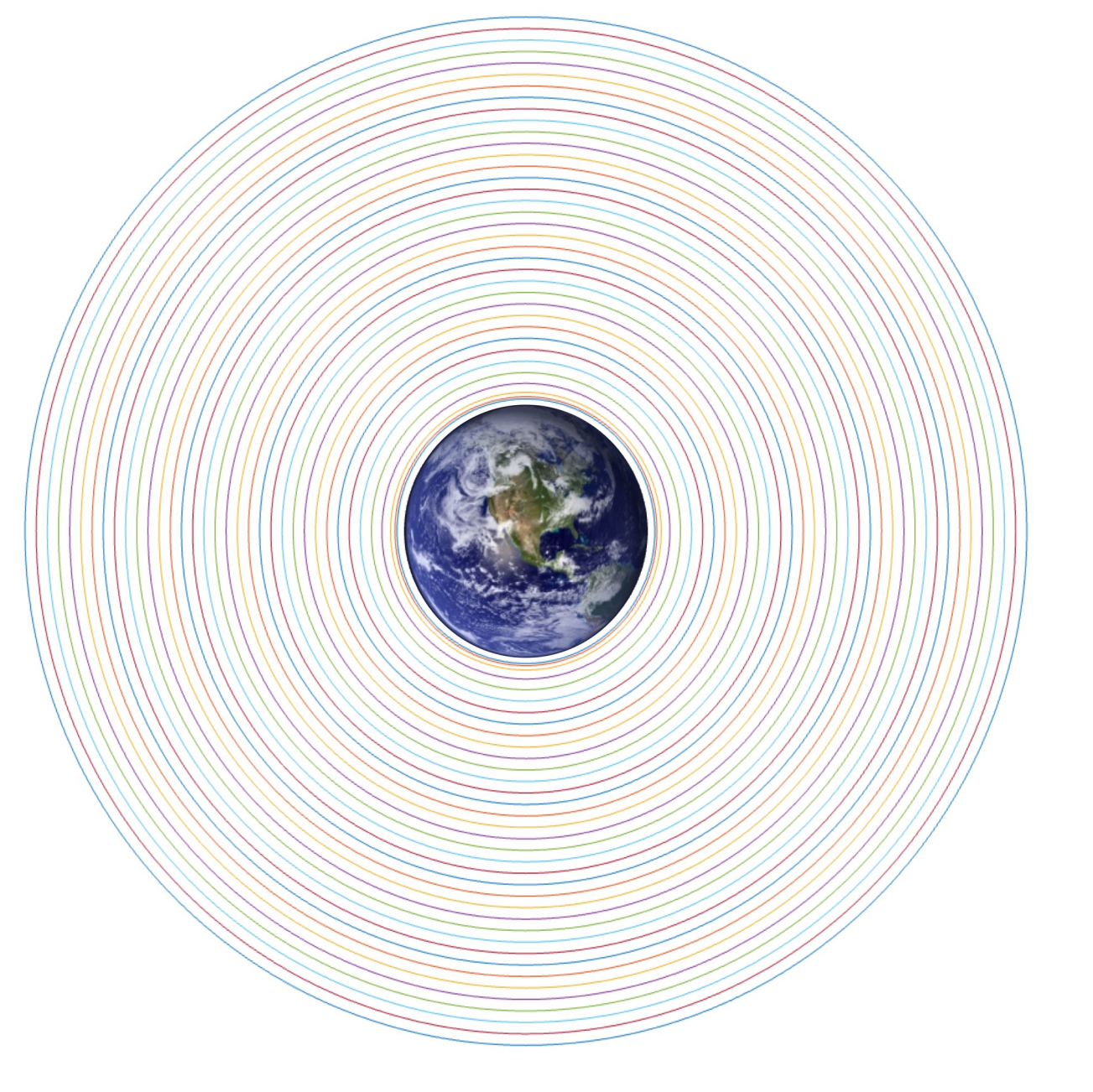


Fig 5. A scale visual of the model shell heights. Output is reported from 400 km to 19940 km.

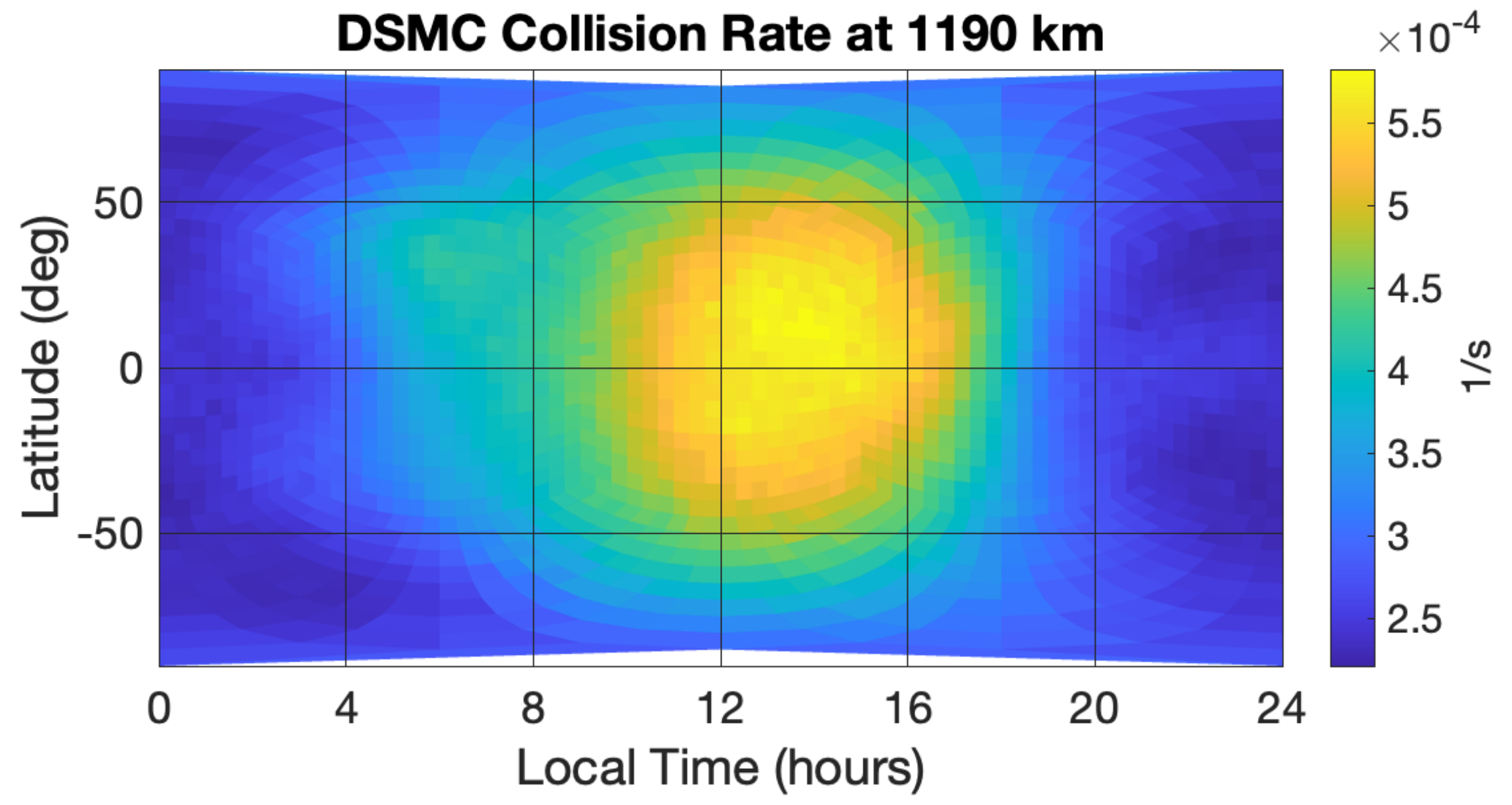


Fig 6. The collision rate of particles is one output of the DSMC model.

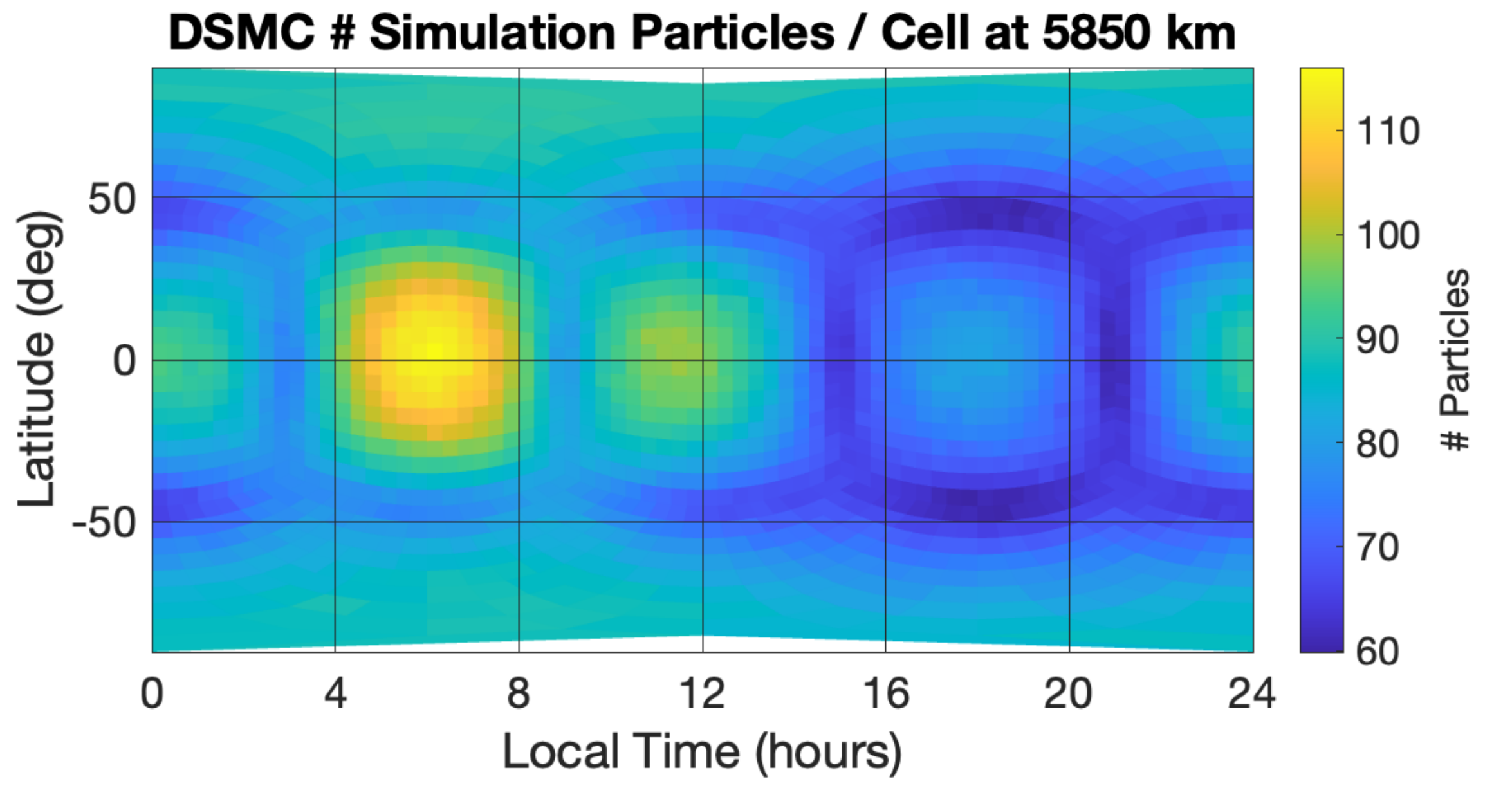
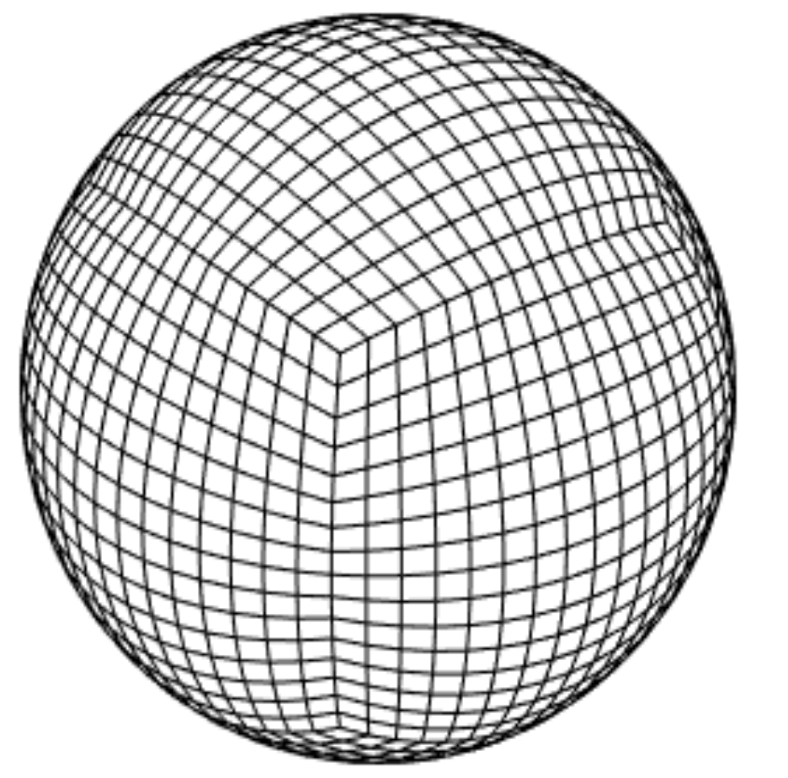


Fig 7. Number of simulation particles in each cell of the simulation grid for a total number density simulation. The structure of the cubed-sphere grid (below) is visible.



Left: Fig 8. A "cubed-sphere" grid forms each layer of cells.

V. Coupling to TIME-GCM

DSMC model lower boundary initial conditions

- Initial conditions are derived from TIME-GCM, a fluid model which extends from 32 km to an altitude ~500 km, depending on solar activity [6].
- The DSMC model takes output from TIME-GCM at 362 km, where the ratio of the mean free path of constituents to the DSMC grid separation is ≤ 1 for both solar minimum and maximum conditions.

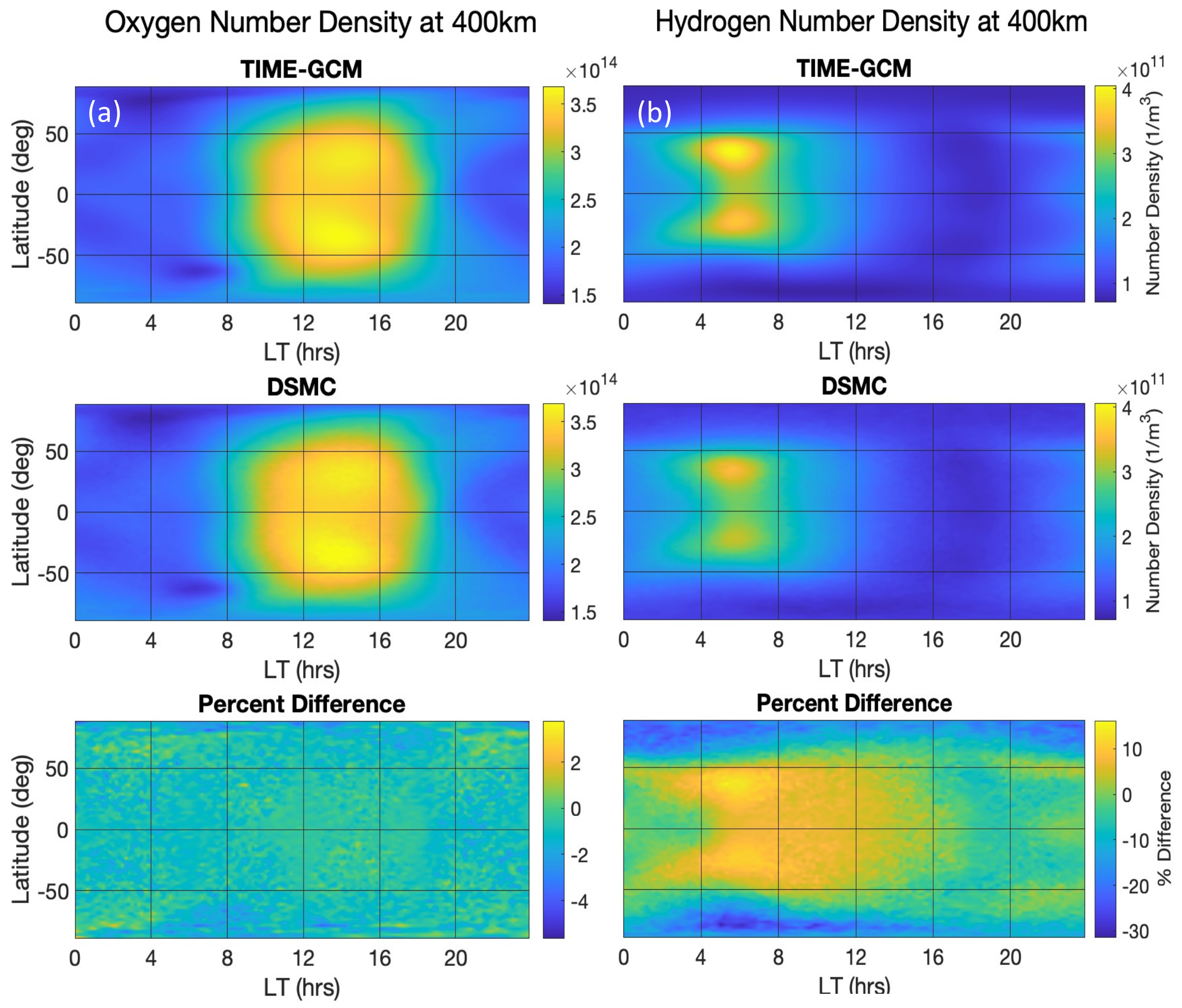


Fig 9. While the number density of N2, O (a), and He in TIME-GCM and the DSMC model agree well at 400 km, the number density of H (b) has up to a 30% difference between the two models at that altitude, requiring further investigation.

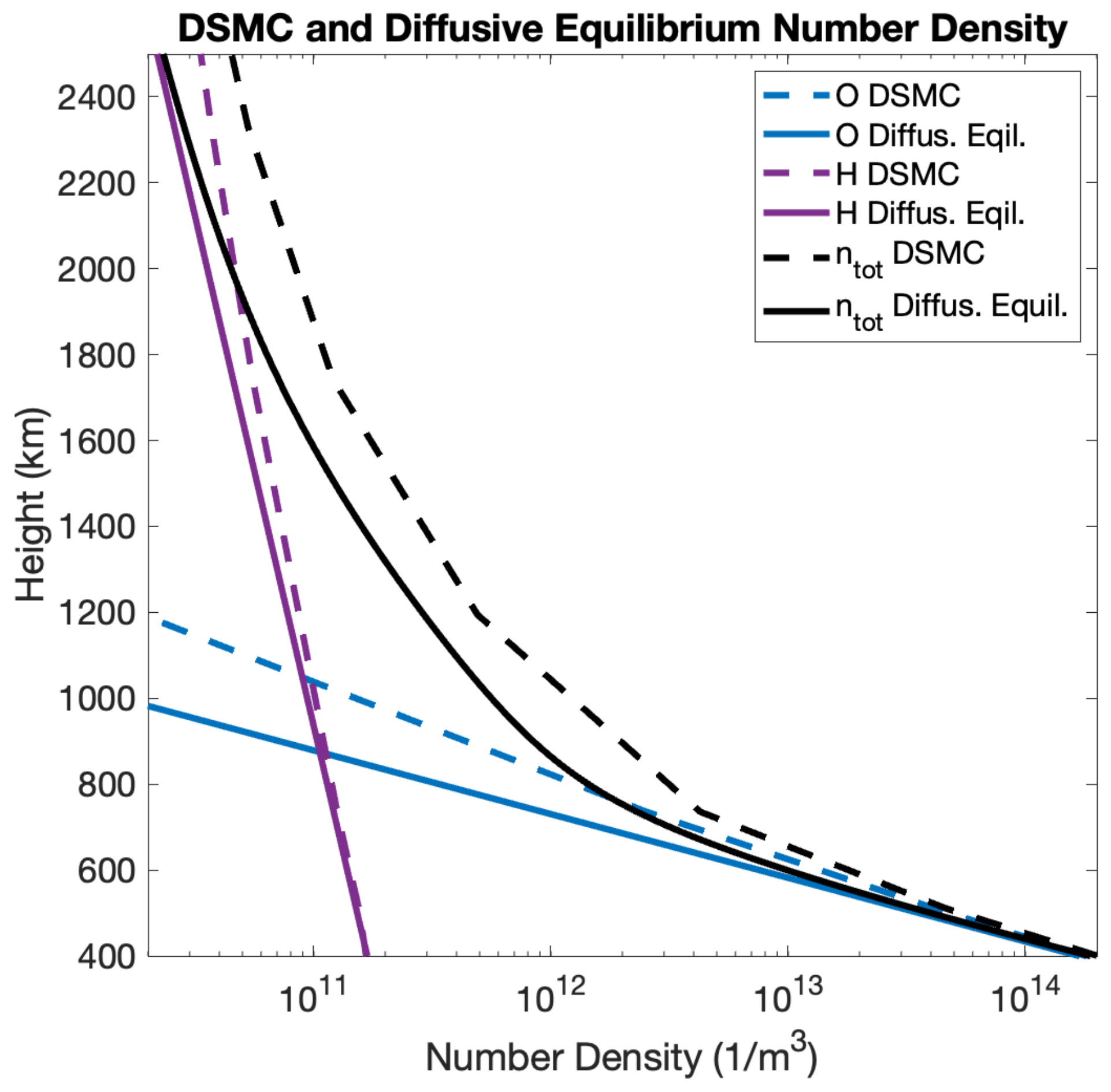


Fig 10. The DSMC model results diverge from the diffusive equilibrium state dictated by the properties of the upper boundary of TIME-GCM.

VI. Future Steps

- Allow exiting ballistic particles to reenter the model upper boundary
- Examine the accuracy of the model at higher altitudes which may be lacking due to the low number of simulation particles
- Perform 2-way coupling
  1. Ensure parameters (especially diffusion coefficients, viscosity coefficients, and density) match at regions where the simulations overlap
  2. Determine how to feed information from DSMC model back into the upper boundary of TIME-GCM

VII. Acknowledgements

Acknowledgements:
The Authors would like to thank Professor Ian Boyd's research group for the development of the DSMC model MONACO, and the NASA FINESST Program for funding support.

Funding :

- NASA FINESST Proposal #20-HELIO20-0005
- NASA HTMS Grant #80NSSC20K1278

VIII. References

[1] Bird, G. (1994*). Molecular Gas Dynamics and the Direct Simulation of Gas Flows*. Claredon Press. ISBN: 0198561954

[2] Bougher, S. et al. (2008). Neutral Upper Atmosphere and Ionosphere Modeling. *Space Science Reviews*, 139(1), 107-141. DOI: 10.1007/s11214-008-9401-9.

[3] Boyd, I. and Schwartzentruber, T. (2017). *Nonequilibrium Gas Dynamics and Molecular Simulation*. Cambridge University Press. DOI: 10.1017/9781139683494.

[4] Chamberlain, J. (1963). Planetary Coronae and Atmospheric Evaporation. *Planetary and Space Science*, 11(8), 901-960. DOI: 10.1016/0032-0633(63)90122-3.

[5] Gallis, M. (2021). DSMC Simulations of Gas Flows. ORNL Project Review, Albuquerque, NM. https://www.osti.gov/servlets/purl/1847485.

[6] High Altitude Observatory (HAO) (2018). TIEGCM V1.94 Model Description. Retrieved from www.hao.ucar.edu/modeling/tgcm/ doc/description/model_description.pdf

[7] Thayer, J., et al. (2021). Remaining Issues in Upper Atmosphere Satellite Drag. In A. Coster, P. Erickson, L. Lanzerotti, Y. Zhang and L. Paxton (Eds.), *Space Weather Effects and Applications* (pp. 111-140). American Geophysical Union. DOI: 10.1002/97811198 15570.ch5