Rarefied gas dynamic simulation of transfer and escape in the Pluto-Charon system with the DSMC method.

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Introduction

Pluto has been observed to support an **extensive, escaping atmosphere**, predominantly composed of nitrogen and methane. Our application of a rarefied gas dynamic technique to simulation of the plutonian upper atmosphere is motivated by ongoing New Horizons data analysis and interpretation[1][9], the extension of plutonian general circulation models (GCMs)[2], and the need for kinetic theory in **predicting and evaluating escape from and transfer within the complex, rarefied Pluto-Charon environs**[3][4].

Here, we apply DSMC in a **three-dimensional, steady-state neutral density model** of Pluto's rarefied upper atmosphere, its escape, and its transfer to Charon.

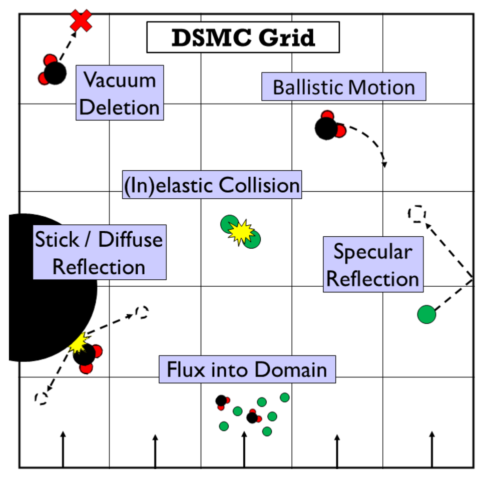
- Comprehensive simulations, featuring hundreds of millions of particles distributed across hundreds of processors, are computed in a hemispherically-symmetric domain spanning from the plutonian exobase to a distant vacuum boundary, inclusive of Charon.

Methodology

The DSMC method is a Lagrangian, particle-based approach applicable to a wide range of **continuum-to-rarefied flows**[5]. Past atmospheric work has applied the technique in simulating the complete Ionian atmosphere[6], and Earth's neutral atmosphere from mid-thermosphere through the exobase[7][8].

- Motions, collisions, and physics of representative molecules are computed, offering a provably probabilistic solution to the Boltzmann equation.
- Mean free path should be comparable to a flow characteristic length scale.
- For planetary atmospheric simulation, this length is the **scale height**.

- In this simulation, representative particles…
  - Are **created** in flux through the lower boundary,
  - Are **moved** by integrating their equations of motion,
  - **Collide** in binary interactions with cell 'partners'.
  - **Escape**, resulting in their deletion, as return flux through the lower boundary or to vacuum. At Charon, particles may either *stick* or *bounce* (diffuse reflection).
- Particles are simulated as variable hard spheres (VHS) with rotational and vibrational states.
- Multispecies flow includes **nitrogen** and **methane**.



Domain Selection

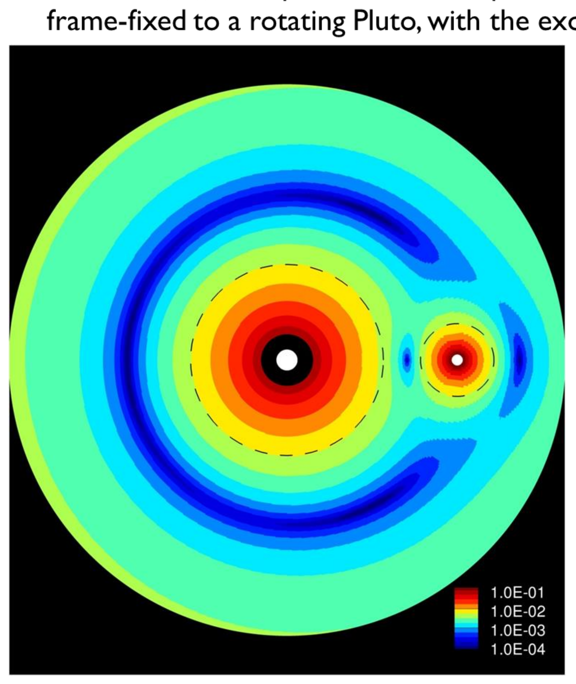
Continuum models break down with steep gradients in flow macroscopic variables, when **characteristic scale length ~ mean free path**.

- Consider the Knudsen number: $Kn = \lambda / L$. The exobase boundary is the location where $Kn = 1.0$ for L the atmospheric scale height, defined here as $kT/m\,g(r)$.
- The DSMC simulation begins below the exobase, between $Kn = 0.1$ and $Kn = 1.0$, at a boundary surface with information generated via a lower-atmospheric model[2].

Pluto and Charon are mutually tidally locked: we consider the problem in a **synodic frame**, in which particles experience fictitious forces accounting for rotation.

- Given an isotropic exobase in number density, concentration, and temperature[1], a **hemispheric symmetry** is enforced via specular reflection across the equatorial plane.

Gradient of effective potential in the equatorial plane for the Pluto-Charon case, frame-fixed to a rotating Pluto, with the exobase drawn at 3000 [km] from center.

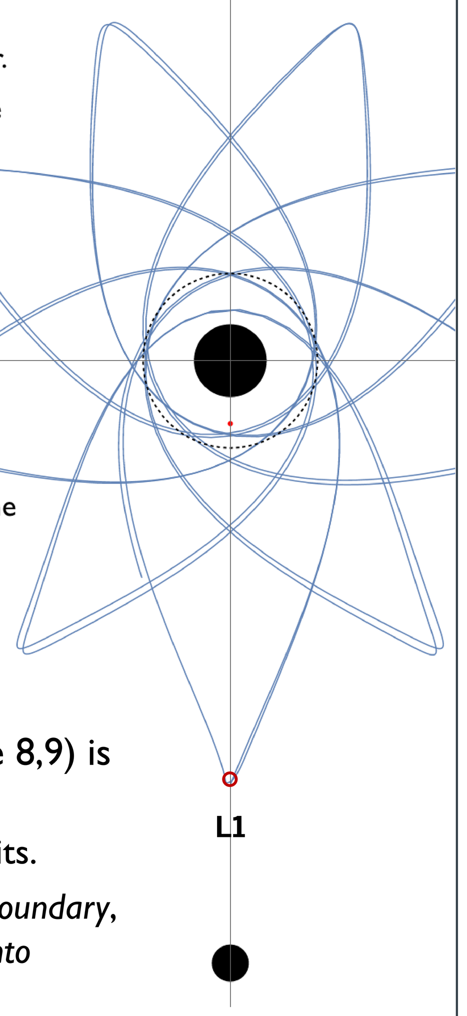


The *Lagrange points* at left are the five evident minima (zeroes) of the field.

```
L1: { 1.38012*10⁷, 0.}
L2: { 2.67254*10⁷, 0.}
L3: {-1.83789*10⁷, 0.}
L4: { 9.78570*10⁶, 1.69493*10⁷}
L5: { 9.78570*10⁶,-1.69493*10⁷}
```

In this case, all are **unstable equilibria**.

Dotted lines indicate the extent of the zones in which orbiting material is effectively gravitationally bound. **Transfer occurs through the L1 Lagrange point.**



Use of a high-order integrator (Runge-Kutta Dormand-Prince 8,9) is motivated by time scales of atmospheric settling…

- *Creation* balanced by *deletion* after **8×10^6 s**, about fifteen orbits.
- Flux in is constant, fluxes out via **a)** *return through the lower boundary*, **b)** *vacuum escape* through the upper boundary, and **c)** *flux onto Charon's surface*. Each settles with a characteristic time-scale.
- Shortest mean time between collisions, near Pluto, is **2×10^2 s.**

… and by a need to resolve the steep gradients in effective potential.

Atmospheric Generation

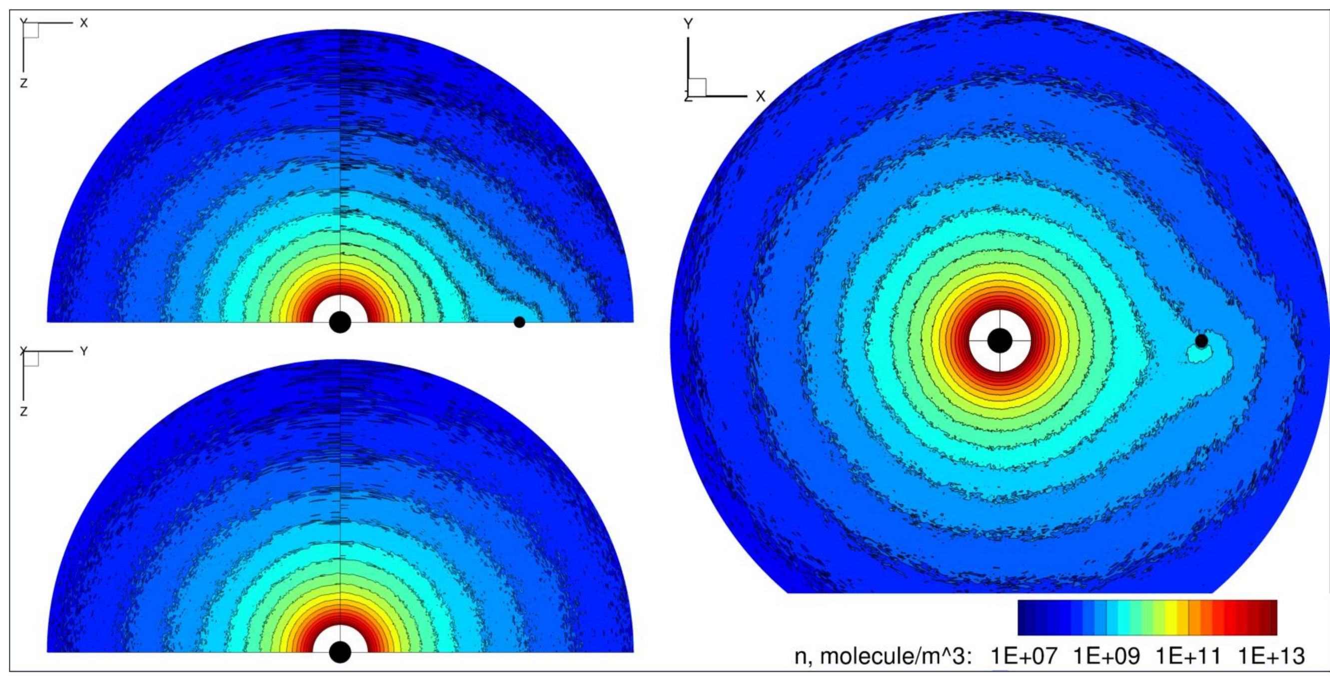
At every timestep, in every boundary cell, for each species [N_2, CH_4]:

[1] Calculate the species' number flux through the surface.
[2] Sample from a Poisson distribution to yield an integer count of particles.
[3] Particles are generated with positions randomly distributed on the lower boundary, with their velocities Maxwellian-distributed.

After an equilibration period, the system achieves a steady state.
With no transient variance in exobase condition, fluxes into and out of the domain balance. Flowfield statistical noise remains to be counteracted with time and ensemble averaging.

Results

Figure 1: A three panel view shows orthogonal cut-planes in contours of total number density. Pluto and Charon are marked in black, and Pluto's collisional atmosphere in white. Both bodies are rotating CCW, and revolving CCW about the barycenter. Note the distortion of the density field under Charon's gravity and the ***transfer*** of escaping atmosphere to a high-density region at Charon's trailing hemisphere.



Initial Conditions: From [2], an isotropic atmosphere generated at 1815 km above Pluto (r=3000 km) with total number density **$1.34\cdot10^{13}$ m^{-3}** and temperature **85.5 K**. From [10], a molar composition of 99.56 % N2 and 0.44 % CH4.

About this three-dimensional simulation:

- Duration of 16 million seconds, or 29 diurnal cycles.
- Performed on the Stampede supercomputer cluster; **240 processors, 50,000 CPU hour duration**.
- Steady flux into domain of O[10^4 #/s]: in steady-state, some **10^8** representative particles occupy the domain at once, while **10^{11}** distinct particles are generated over the total simulation.

Table 1: The exobase parameters as calculated in this simulation vs. those observed by New Horizons, and (*) the minimum solar-heating case via free-molecular study in [3].

	Exobase Radius	T [K]	Density [#/m³]	N_2 [#/m³]	CH_4 [#/m³]	Jeans [λ]
Simulation Result:	2.59 R_P / 3070 km	85.5	$9.10\cdot10^{12}$	$9.04\cdot10^{12}$	$5.46\cdot10^{10}$	11.2
New Horizons [9] :	2.36 R_P / 2800 km	70.0	$7–12\cdot10^{12}$	$4–7\cdot10^{12}$	$3–5\cdot10^{12}$	12.2
** Tucker et al. [3] :*	5.30 R_P / 6095 km	87.0	$7.00\cdot10^{11}$	$7.00\cdot10^{11}$	--	5.7

Figure 2: (L) 3-D representation of the computed flowfield, highlighting number densities about Charon and demonstrating system geometry.

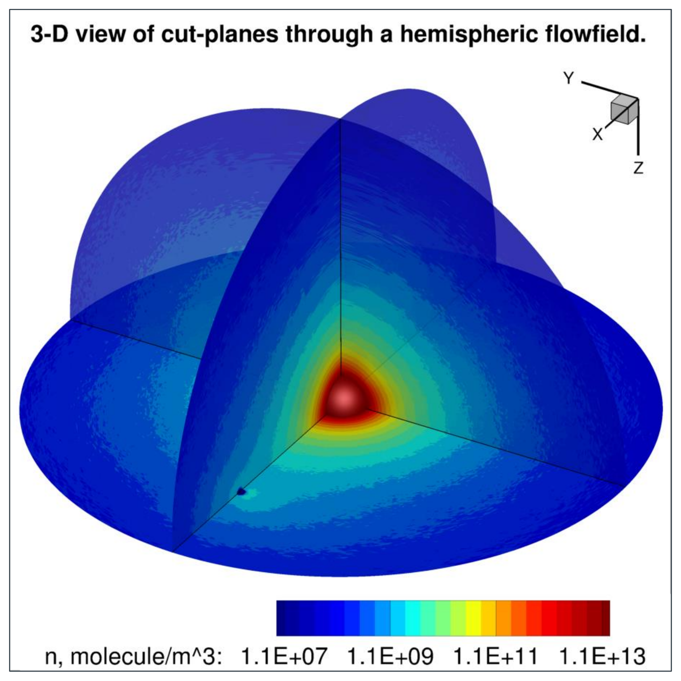


Figure 3: (R) In the simulations shown, particles that strike Charon stick, and are stored. Shown here are rates of deposition on Charon's surface and the fraction of methane in the deposited material (~10%).

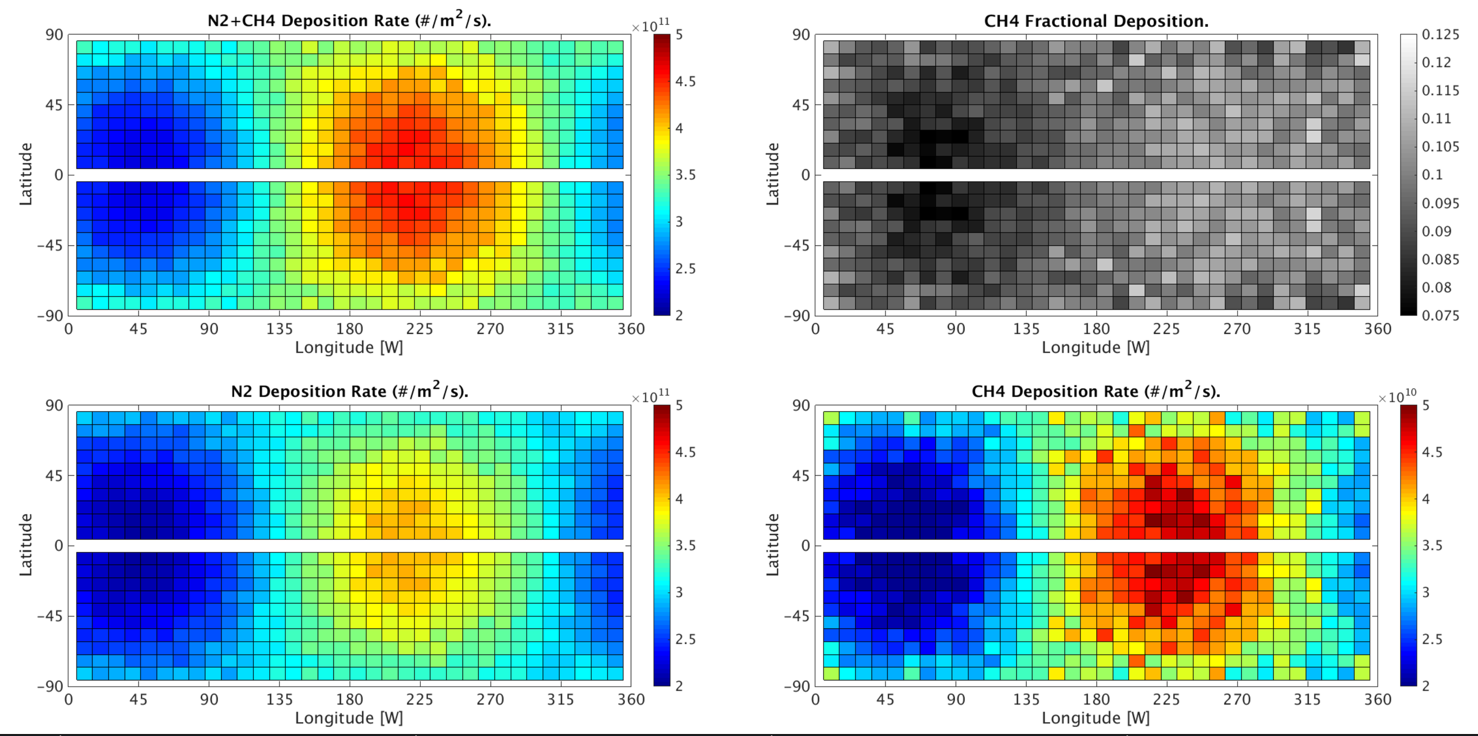
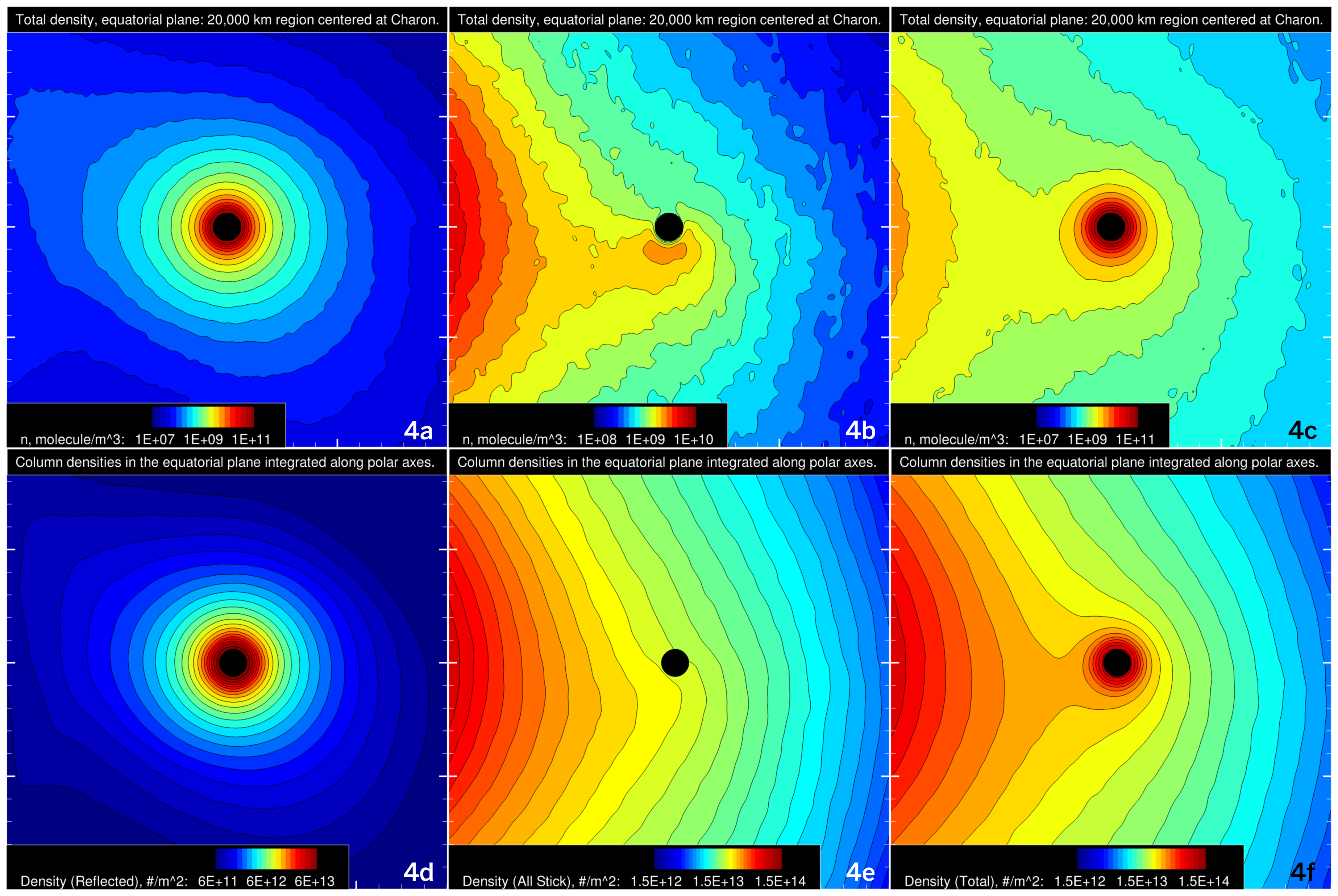


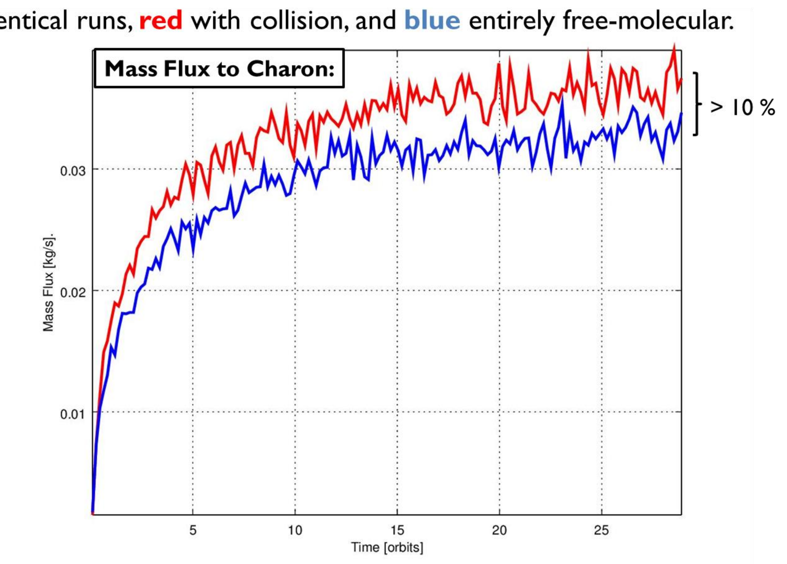
Table 2: Steady-state rates of molecule flux into and out of the domain, including simulated vacuum escape and species flux to Charon.

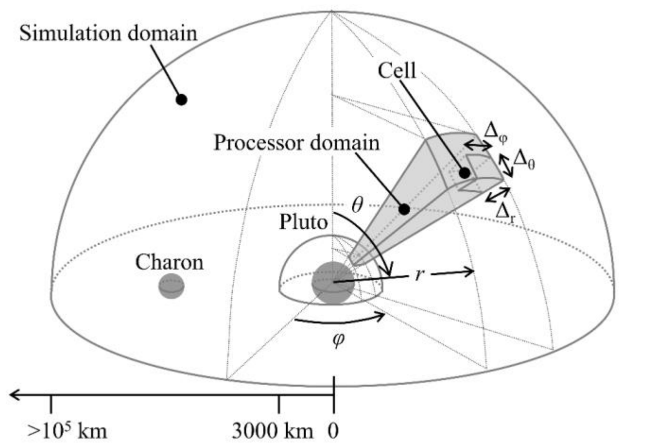
All in [#/s].	Boundary [In]	Boundary [Out]	Vacuum Escape	To Charon: N_2	To Charon: CH_4
Simulation Result:	$9.644\cdot10^{28}$	$9.630\cdot10^{28}$	$3.6–4.2\cdot10^{25}$	$1.40–1.46\cdot10^{24}$	$1.56–1.62\cdot10^{23}$
New Horizons [9] :	--	--	$5.0\cdot10^{25}$	--	--
** Tucker et al. [3] :*	$2.3\cdot10^{28}$	--	$1.2\cdot10^{27}$	$5.7\cdot10^{25}$	--

Figure 4: Now, particles stored at Charon are re-emitted as though they had diffusely reflected from a 53 K uniform surface, and continue to reflect at this temperature. The resultant flow is sufficiently rarefied as to be non-collisional, and may be superimposed with a result in which all particles stick to Charon. Figures 4(*a-f*) show a square region of 20,000 km centered at Charon. The top row of figures (*a-c*) show number densities, while the bottom row (*d-f*) show column densities integrated along the polar axis. At left (*a, d*) are particles which have struck and reflected off Charon alone; at center (*b, e*) the result for the flowfield in which all particles stick to Charon and are effectively deleted; and at right (*c, f*) is the super-imposition. A ***diffuse transfer structure from Charon back toward Pluto*** is evident in the reflected particles, while the near-Charon regime highlights the shape of the gas transfer structure arcing through the L1 point. If particles are permitted to bounce off of Charon, this result suggests that a thin atmosphere could persist on the moon, an ***atmosphere shared between bodies*** in a binary system.



How significant are collisions in generating / directing flux to Charon? Identical runs, red with collision, and blue entirely free-molecular.





The complete hemispheric domain, exhibiting the Pluto-centric spherical reference frame.

Conclusions

A fully three-dimensional model of the steady-state, rarefied component of Pluto's neutral upper atmosphere is presented. Results for **exobase parameters** and **rates of escape to vacuum and transfer** to Charon are compared against a case in the literature, and against the observations of New Horizons, matching well with the latter.

Novel gas-transfer structures are noted in a **binary atmospheric configuration**, including a preferential transfer of material from Pluto's escaping atmosphere to Charon's trailing hemisphere, peaking at 225° W along the equator, and, in the event of total diffuse reflection from Charon, a returning flux preferentially directed toward Pluto's trailing hemisphere.

Charon is shown to be **capable of supporting a thin atmosphere** at column densities as high as $1.5\cdot10^{14}$ m^{-2} in simulations with a plutonian exobase condition similar to that observed by New Horizons.

[1] Stern, S.A. et al. (2015) Science, 350, aad1815 (8 pp). [2] Tucker, O.J., Erwin, J.T., Deighan, J.I., Volkov, A.N., Johnson, R.E. (2012) Icarus, 217, 408–415. [3] Tucker, O.J., Johnson, R.E., Young, L.A. (2015) Icarus, 246, 291-297. [4] Volkov, A.N., Johnson, R.E., Tucker, O.J., Erwin, J.T. (2011) Astrophys. J. Lett. 729:L24 (5 pp). [5] Bird, G.A. (1994) Molecular Gas Dynamics and the Direct Simulation of Gas Flows. Oxford Univ. Press, New York. [6] Walker, A.C., et al. (2010) Icarus, 207, 409–432. [7] Hoey, W.A. et al. (2014) 47th AGU Fall Meeting, Abstract 22218. [8] Hoey, W.A. et al. (2015) DSMC Conference 2015, Abstract: On the Simulation of Rarefied Planetary Atmospheres with the DSMC Method. [9] Gladstone, G.R. et al. (2016) Science, 351, aad8866 (6 pp). [10] Young, L.A., et al. (1997) Icarus, 127, 258-262.