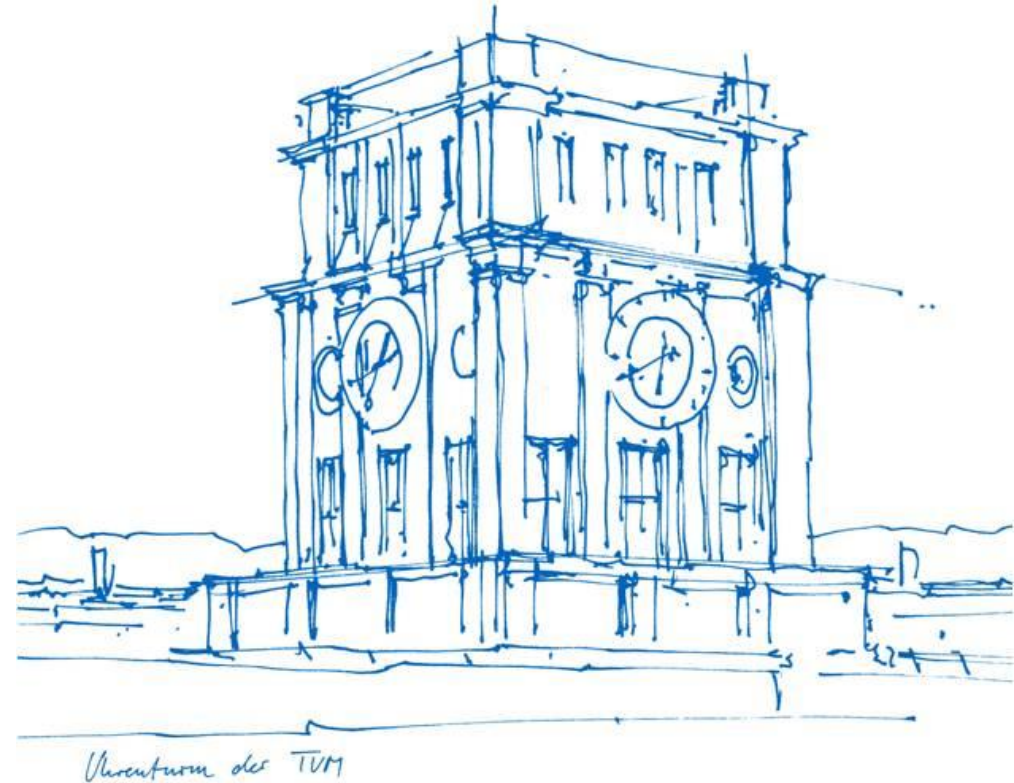


Extraterrestrial Exosphere and Surface Simulations

Lunar Water Exosphere



Alexander Smolka

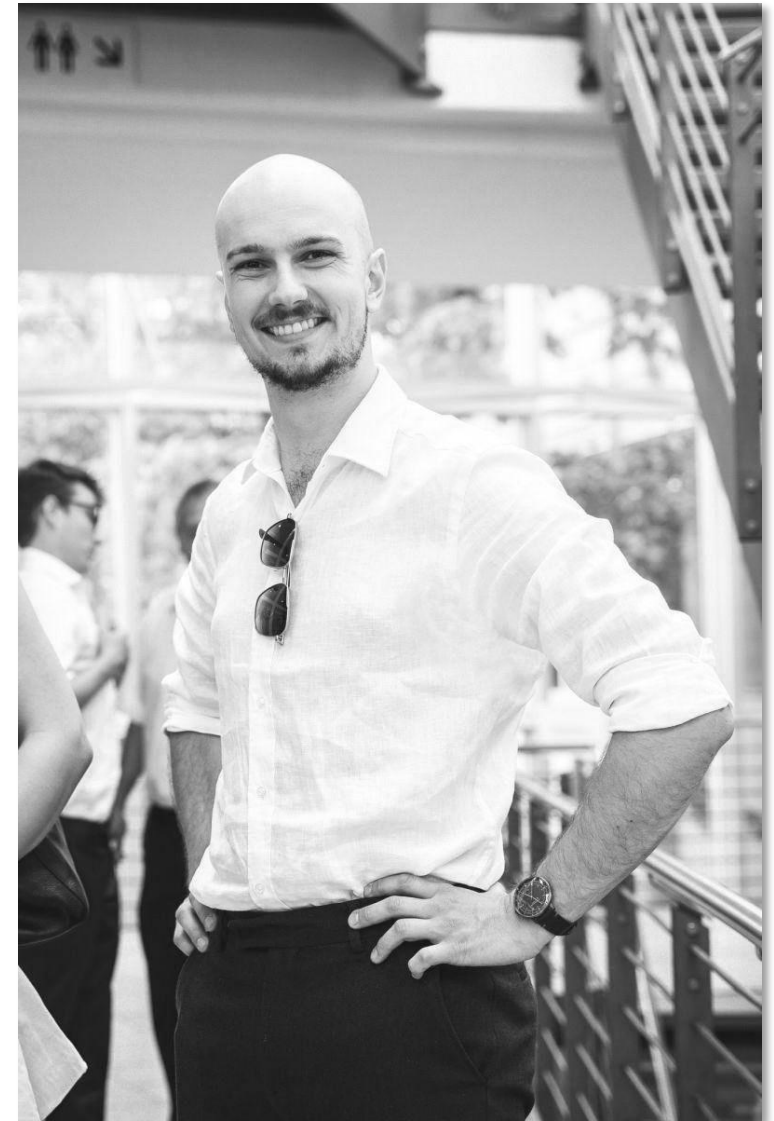
*Lunar and Planetary Exploration
Technical University of Munich*



Alexander Smolka

Researcher, Technical University of Munich, Lunar and Planetary Exploration

-  Research Topic: *Modelling of the Lunar Water Exosphere and its Interaction with the Surface*
-  Methodology: *Numerical simulations using our specially developed high-performance Julia code base.*



Alexander Smolka

B.Sc. in Mechanical Engineering, RWTH Aachen
University

M.Sc. in Aerospace, Technical University of Munich

Researcher, Technical University of Munich, Lunar
and Planetary Exploration



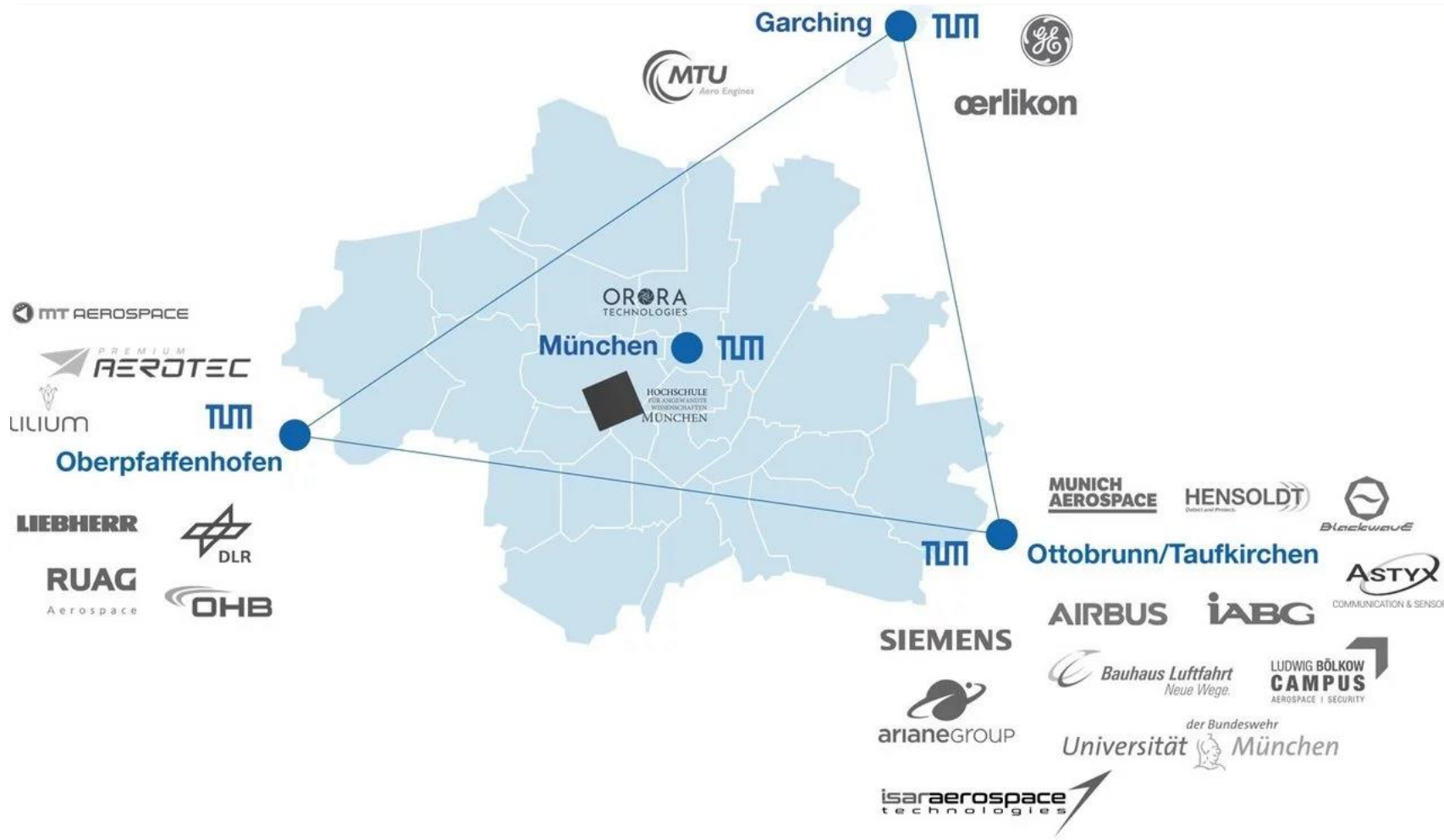
Research Topic: *Modelling of the Lunar Water Exosphere
and its Interaction with the Surface*



Methodology: *Numerical simulations using our specially
developed high-performance Julia code base.*



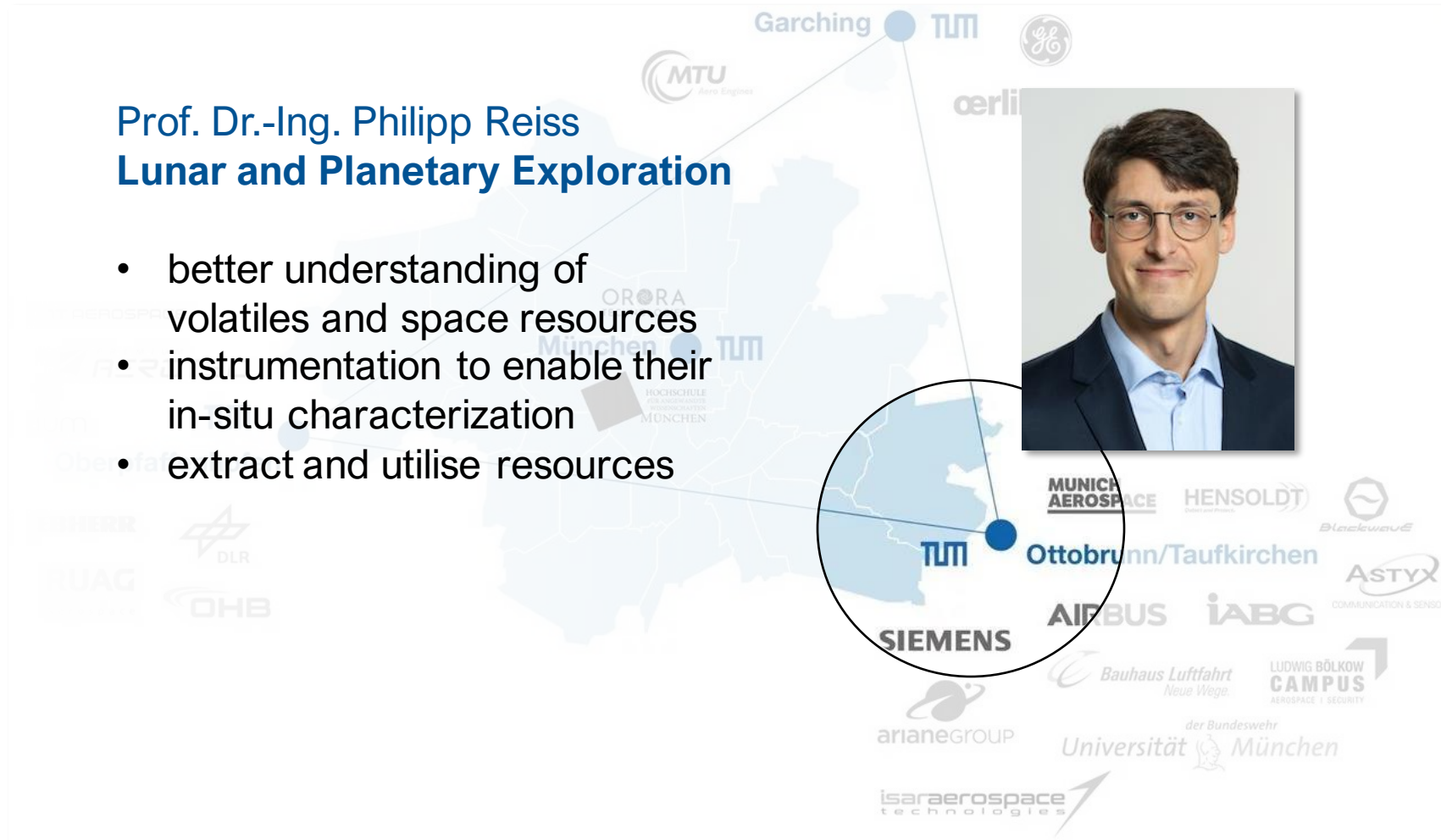
Technical University of Munich



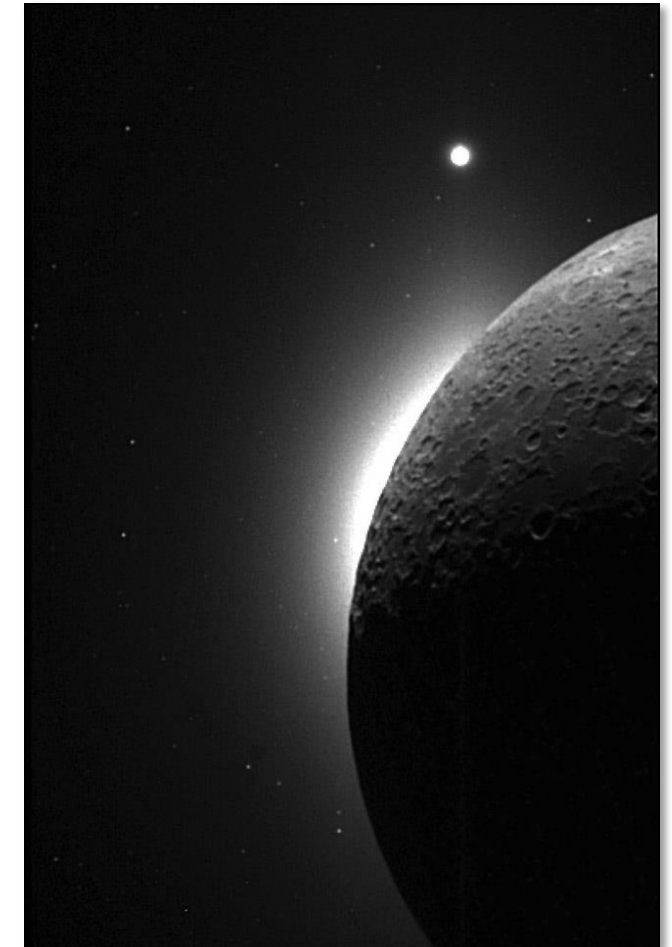
Technical University of Munich

Prof. Dr.-Ing. Philipp Reiss
Lunar and Planetary Exploration

- better understanding of volatiles and space resources
- instrumentation to enable their in-situ characterization
- extract and utilise resources



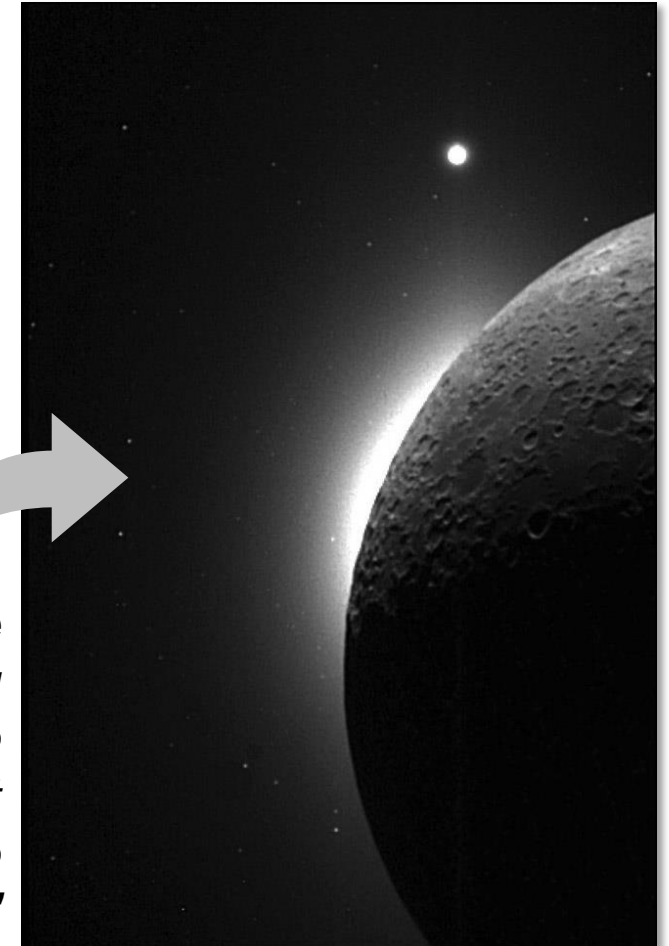
The Lunar Exosphere



(Image credit: NASA)

The Lunar Exosphere

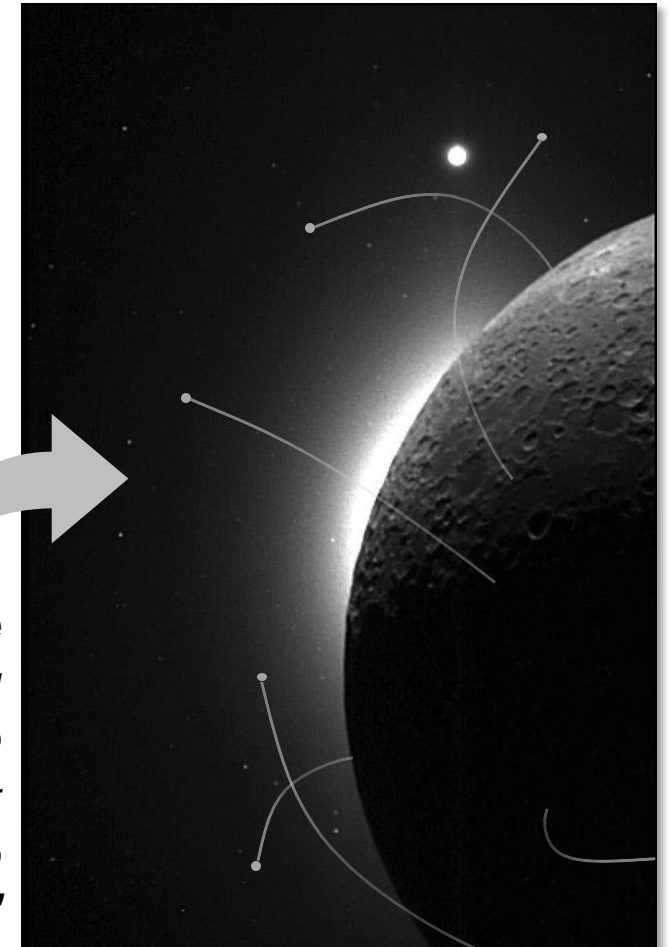
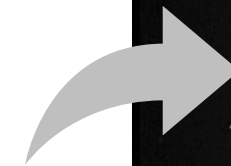
Surface-bounded Exosphere
"[...] atmosphere-like volume surrounding a planet [...] where molecules are gravitationally bound to that body, but where the density is so low that the molecules are essentially collision-less."



(Image credit: NASA)

The Lunar Exosphere

Surface-bounded Exosphere
"[...] atmosphere-like volume surrounding a planet [...] where molecules are gravitationally bound to that body, but where the density is so low that the molecules are essentially collision-less."

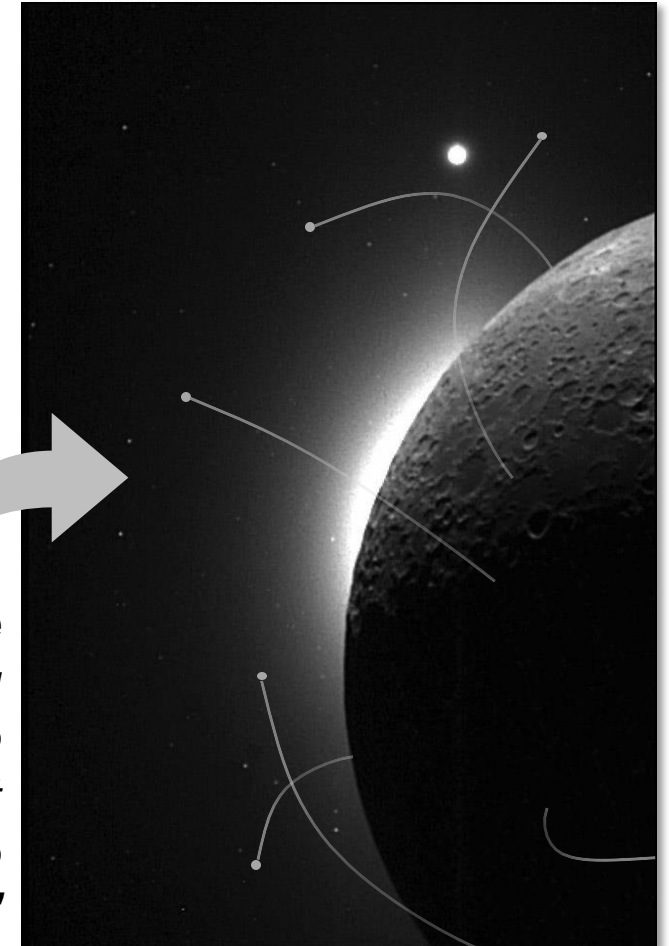


(Image credit: NASA)

The Lunar Exosphere

*We can
simulate them
individually!*

Surface-bounded Exosphere
*"[...] atmosphere-like volume surrounding
a planet [...] where molecules are
gravitationally bound to that body, but
where the density is so low that the
molecules are essentially collision-less."*



(Image credit: NASA)

The Lunar Exosphere

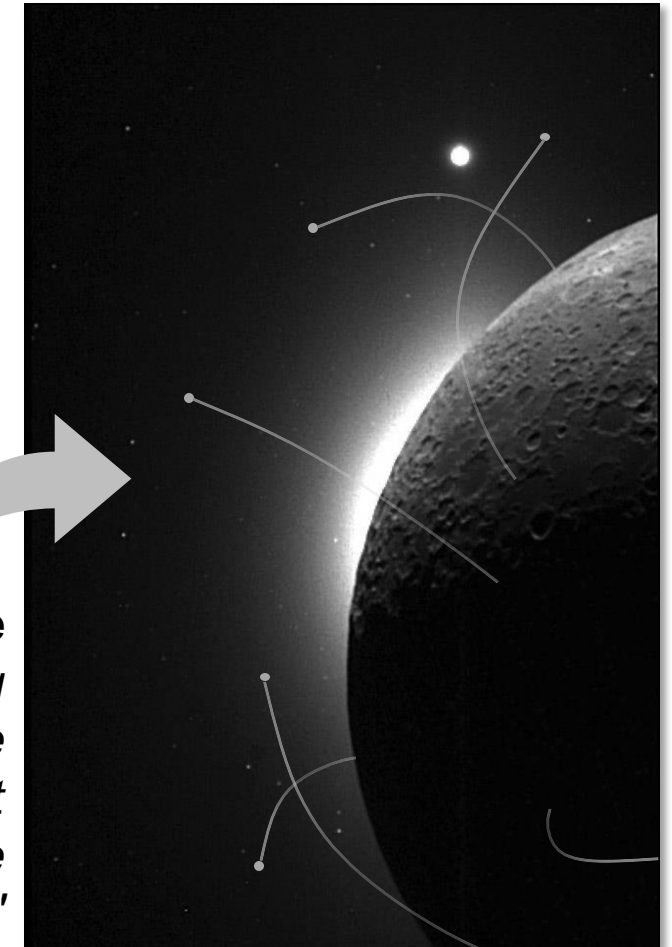
Densities are highly dependent on the position (equatorial/polar) and time (day/night)!

H	$\sim 1 - 10 \text{ cm}^{-3}$
H ₂	$\sim 100 - 10^4 \text{ cm}^{-3}$
He	$\sim 100 - 5 \times 10^4 \text{ cm}^{-3}$
OH	$\sim 1 \text{ cm}^{-3}$
H ₂ O	$\sim 1 - 10^3 \text{ cm}^{-3}$
Ne	$\sim 10^3 - 10^5 \text{ cm}^{-3}$
...	...

Comparison with Earth's atmosphere:
 $2.687 \times 10^{19} \text{ cm}^{-3}$

We can simulate them individually!

Surface-bounded Exosphere
 "[...] atmosphere-like volume surrounding a planet [...] where molecules are gravitationally bound to that body, but where the density is so low that the molecules are **essentially collision-less.**"



(Image credit: NASA)

The Lunar Exosphere

Densities are highly dependent on the position (equatorial/polar) and time (day/night)!

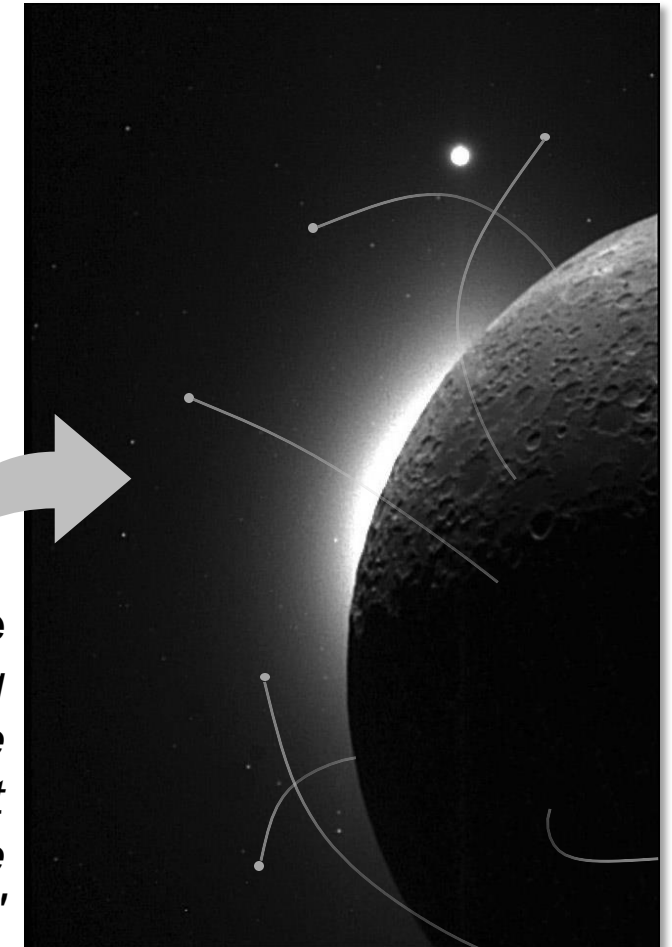
H	$\sim 1 - 10 \text{ cm}^{-3}$
H ₂	$\sim 100 - 10^4 \text{ cm}^{-3}$
He	$\sim 100 - 5 \times 10^4 \text{ cm}^{-3}$
OH	$\sim 1 \text{ cm}^{-3}$
H ₂ O	$\sim 1 - 10^3 \text{ cm}^{-3}$
Ne	$\sim 10^3 - 10^5 \text{ cm}^{-3}$
...	...

We cannot simulate all of them!

We can simulate them individually!

Comparison with Earth's atmosphere:
 $2.687 \times 10^{19} \text{ cm}^{-3}$

Surface-bounded Exosphere
 "[...] atmosphere-like volume surrounding a planet [...] where molecules are gravitationally bound to that body, but where the density is so low that the molecules are **essentially collision-less.**"



(Image credit: NASA)

The Lunar Exosphere

Densities are highly dependent on the position (equatorial/polar) and time (day/night)!

H	$\sim 1 - 10 \text{ cm}^{-3}$
H ₂	$\sim 100 - 10^4 \text{ cm}^{-3}$
He	$\sim 100 - 5 \times 10^4 \text{ cm}^{-3}$
OH	$\sim 1 \text{ cm}^{-3}$
H ₂ O	$\sim 1 - 10^3 \text{ cm}^{-3}$
Ne	$\sim 10^3 - 10^5 \text{ cm}^{-3}$
...	...

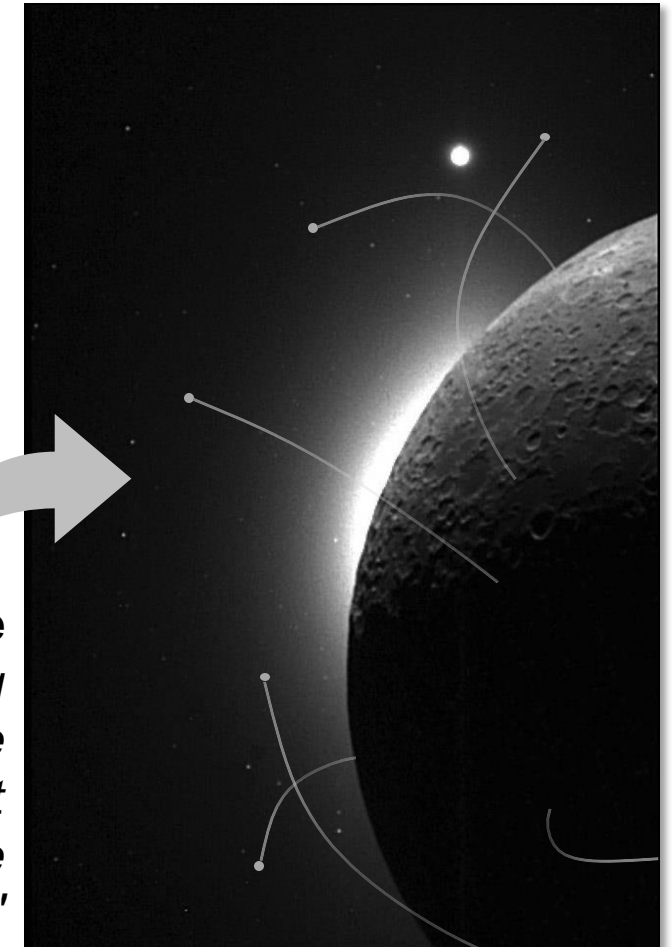
We cannot simulate all of them!

Monte Carlo simulation

We can simulate them individually!

Comparison with Earth's atmosphere:
 $2.687 \times 10^{19} \text{ cm}^{-3}$

Surface-bounded Exosphere
 "[...] atmosphere-like volume surrounding a planet [...] where molecules are gravitationally bound to that body, but where the density is so low that the molecules are **essentially collision-less.**"



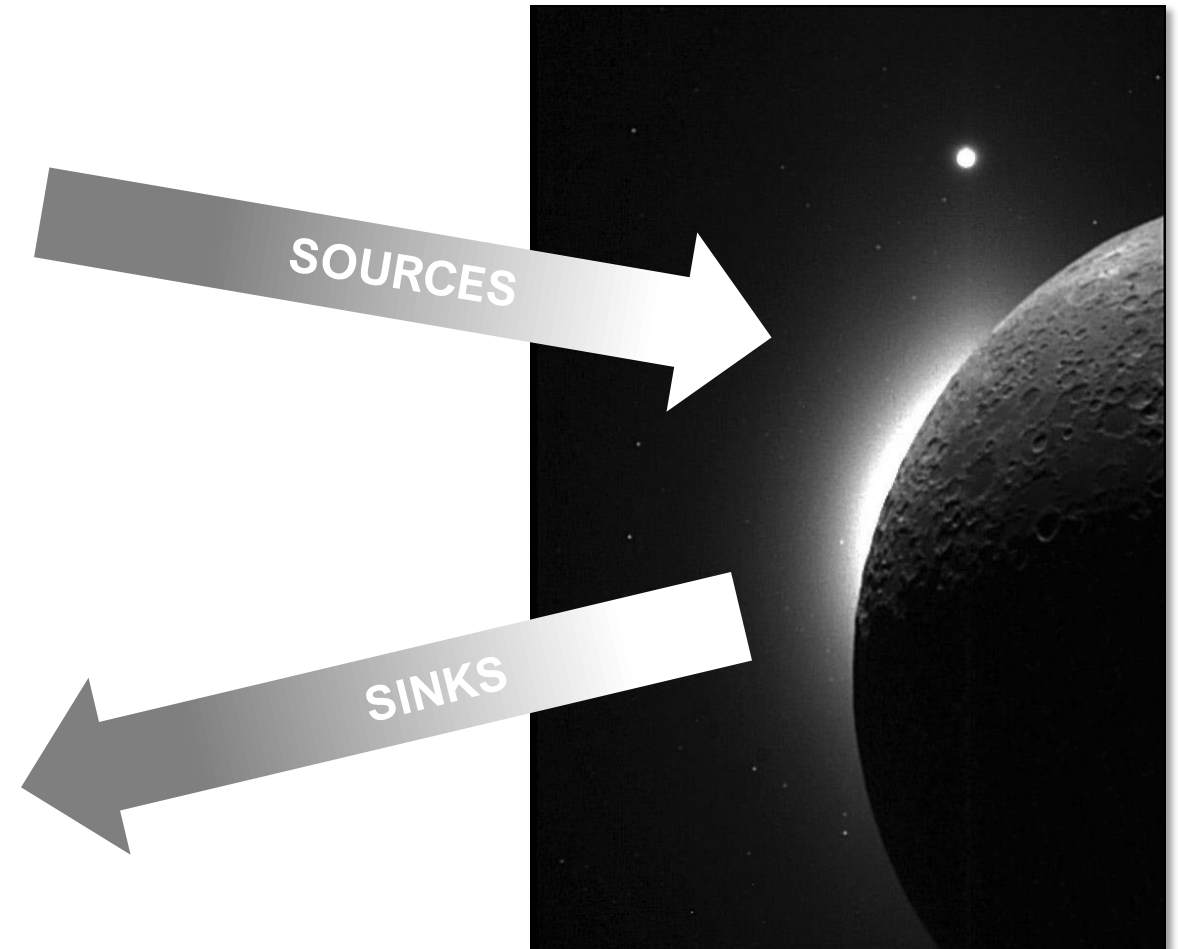
(Image credit: NASA)

The Lunar Exosphere

Sources & Sinks

- Solar wind
- Micrometeoroid Impact
- Micrometeoroid Impact Vaporization
- Sputtering

- Gravitational Escape
- Photolysis
- Sputtering
- Permanent Cold Trapping



(Image credit: NASA)

The Lunar Exosphere

Sources & Sinks

- Solar wind
- Micrometeoroid Impact
- Micrometeoroid Impact Vaporization
- Sputtering

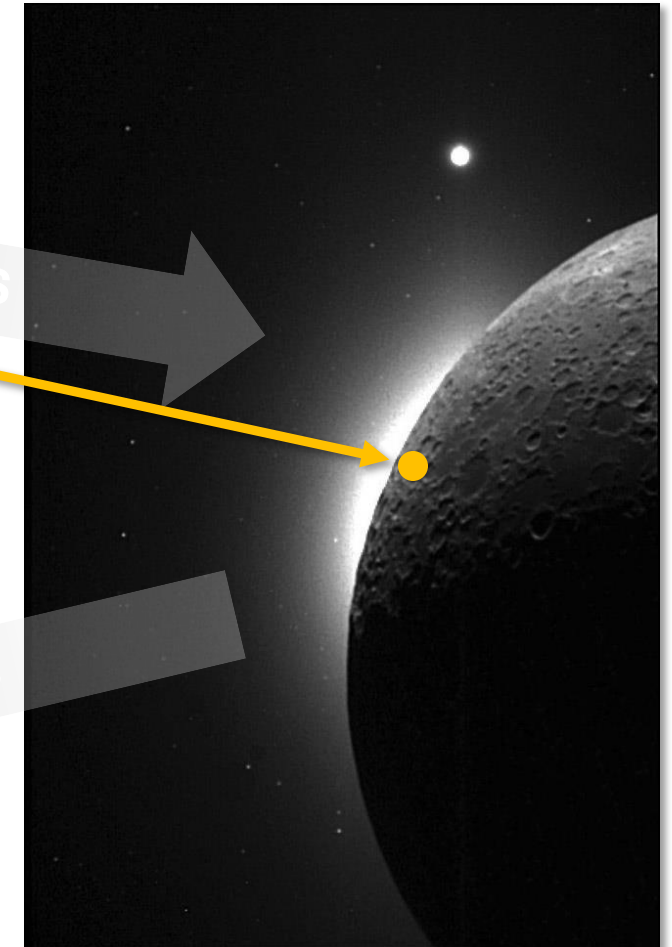
Ions:
 ≈ 96%: p^+
 ≈ 4%: He^{++}

IMPLANTATION

SOURCES

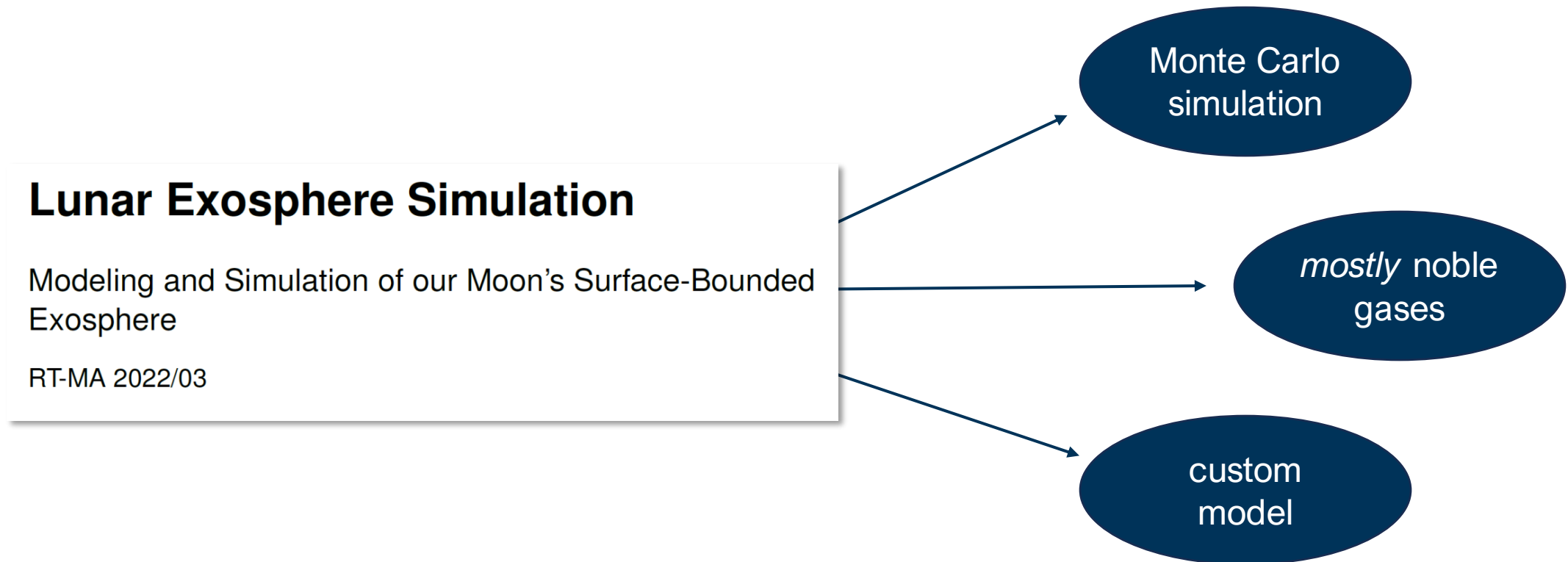
- Gravitational Escape
- Photolysis
- Sputtering
- Permanent Cold Trapping

SINKS

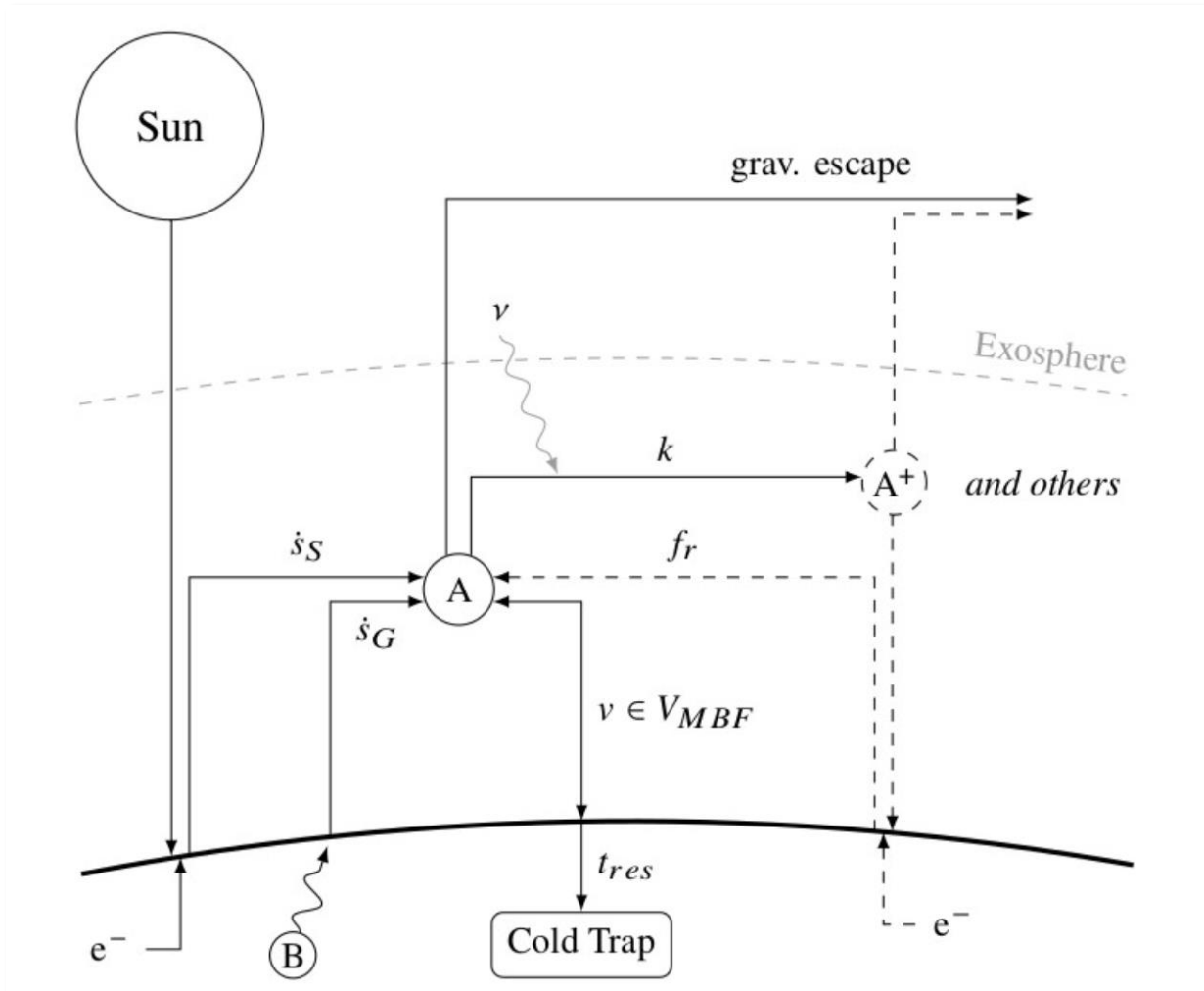


(Image credit: NASA)

Lunar Exosphere Simulation



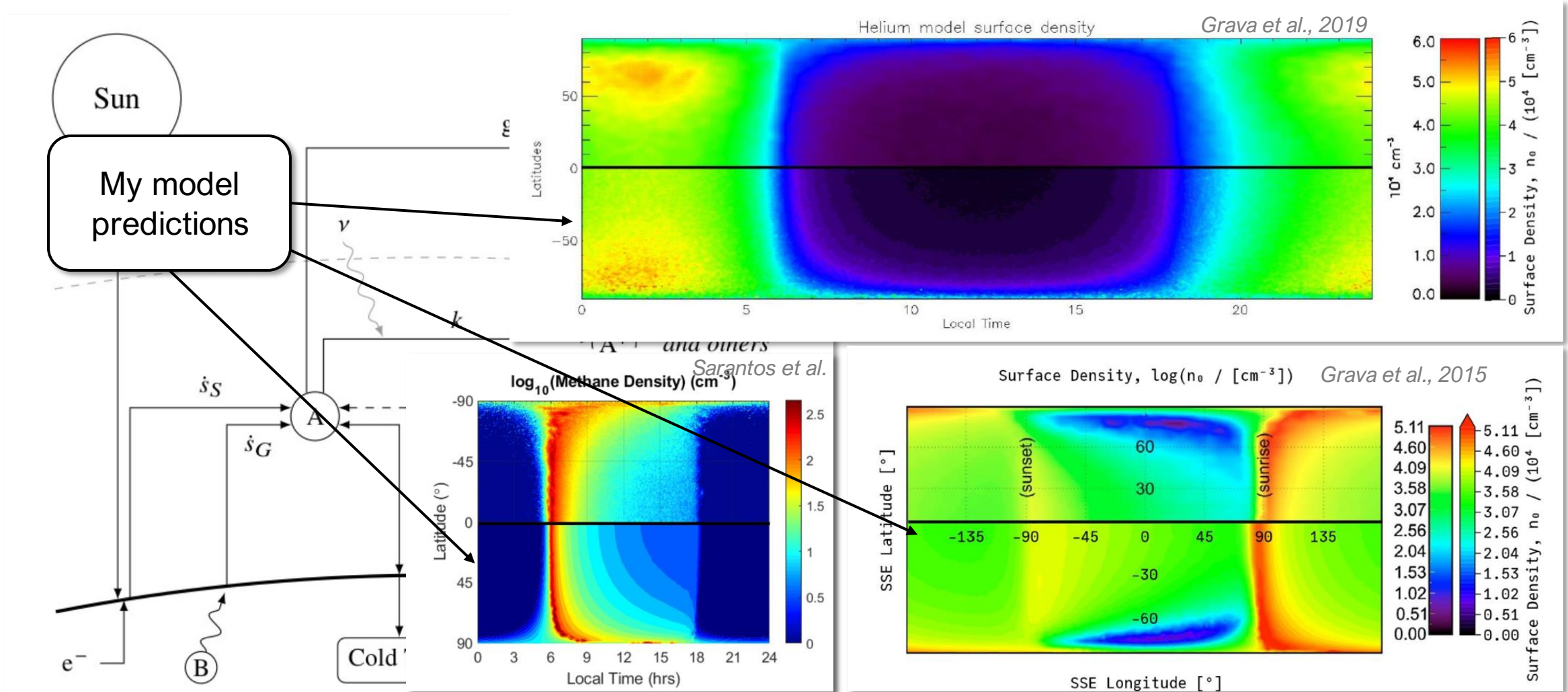
Lunar Exosphere Simulation



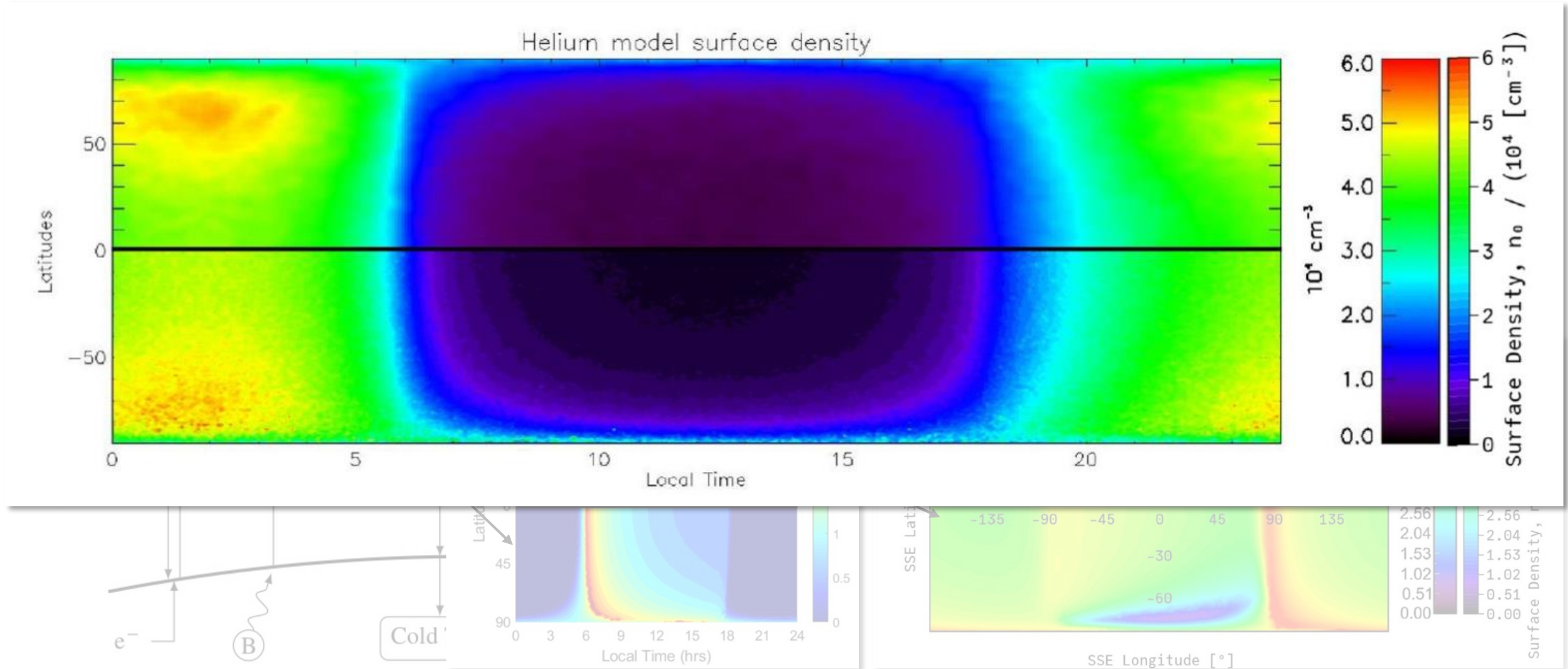
Assumptions:

- 2D landing position calculation instead of 3D ODE trajectory solver
- Only neutral gases
 - Only gravity
- Steady-state conditions without Earth's influence
- ...

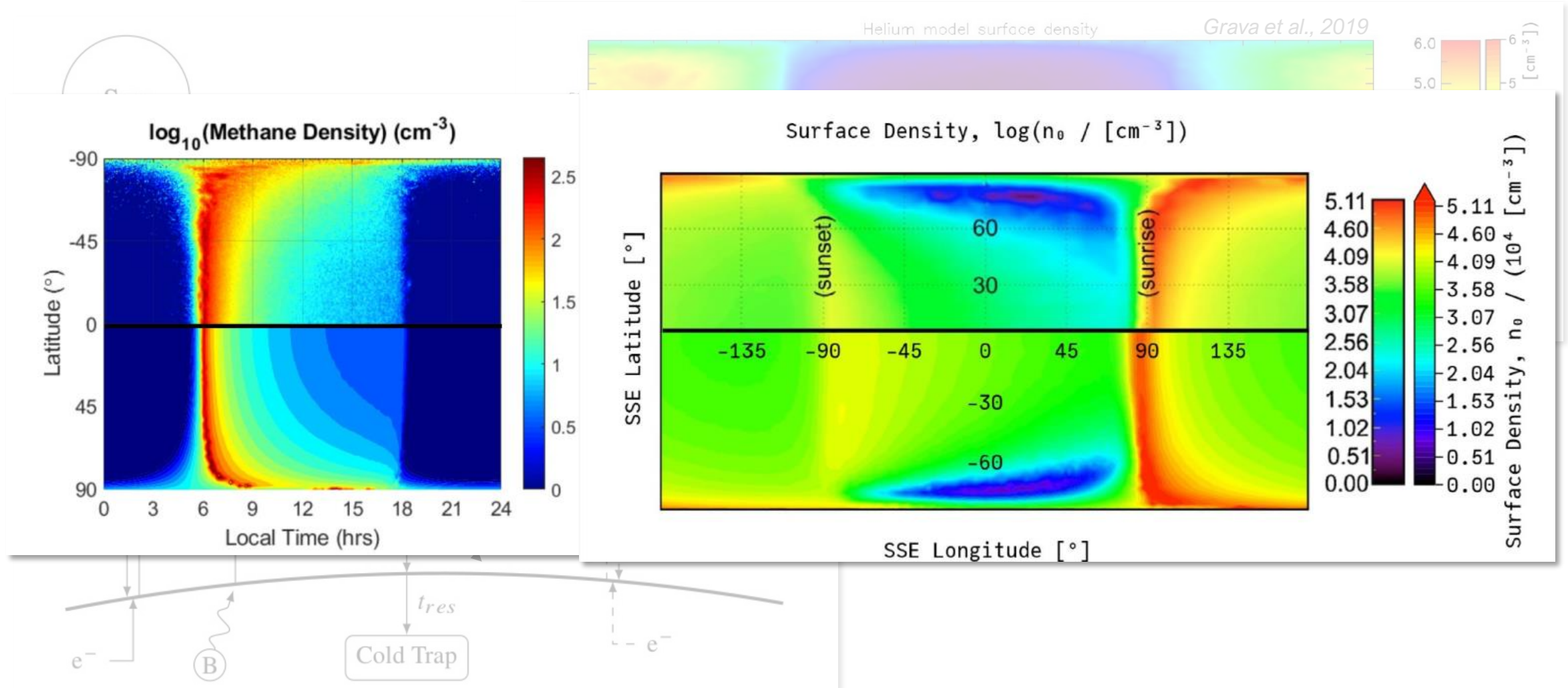
Lunar Exosphere Simulation



Lunar Exosphere Simulation



Lunar Exosphere Simulation



Lunar Exosphere Simulation

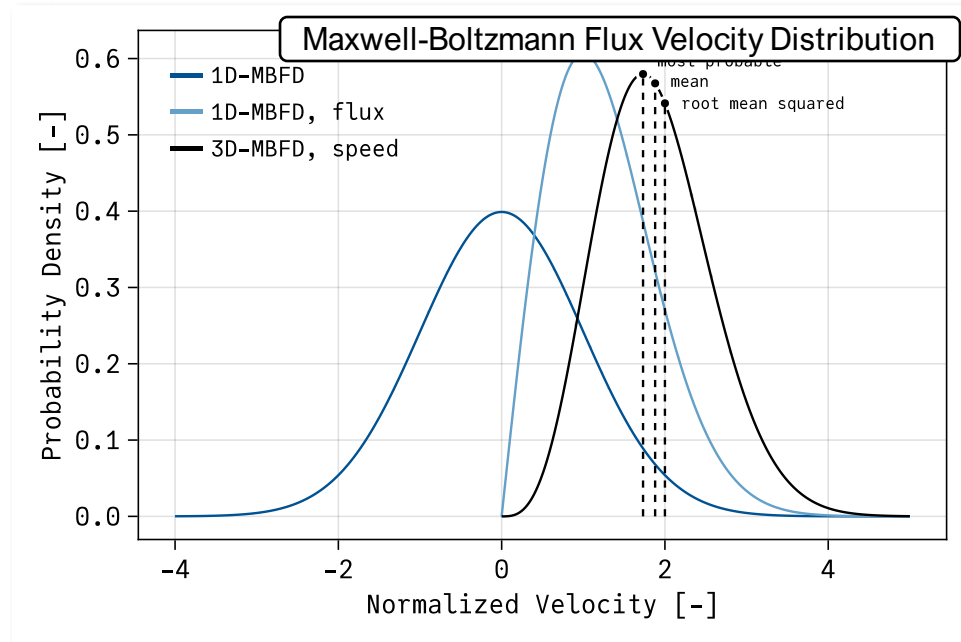
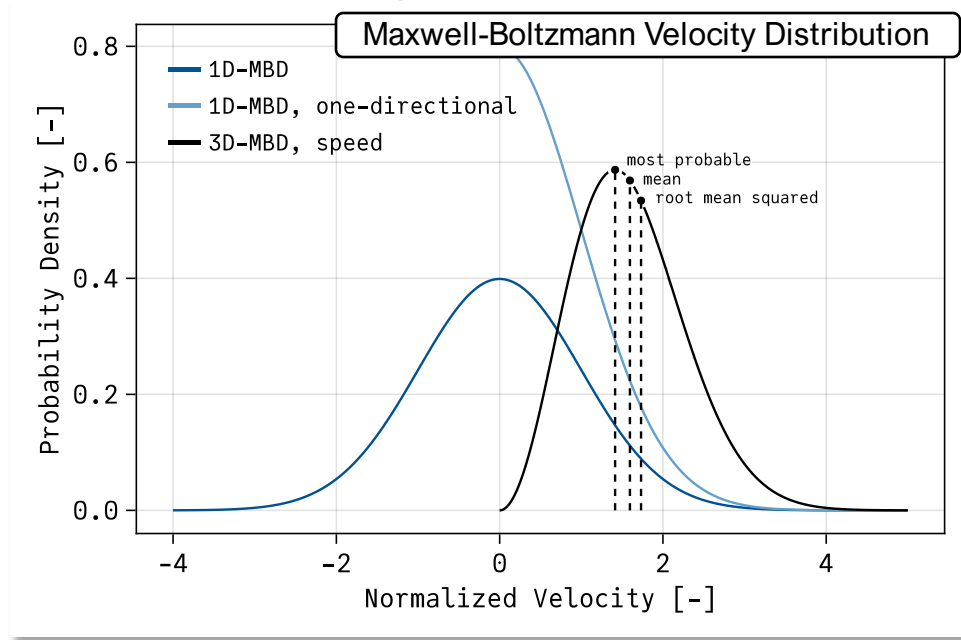
Lunar Exosphere Simulation

Modeling and Simulation of our Moon's Surface-Bounded Exosphere

RT-MA 2022/03

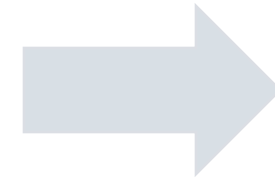


Velocity distributions

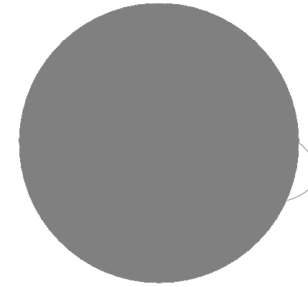
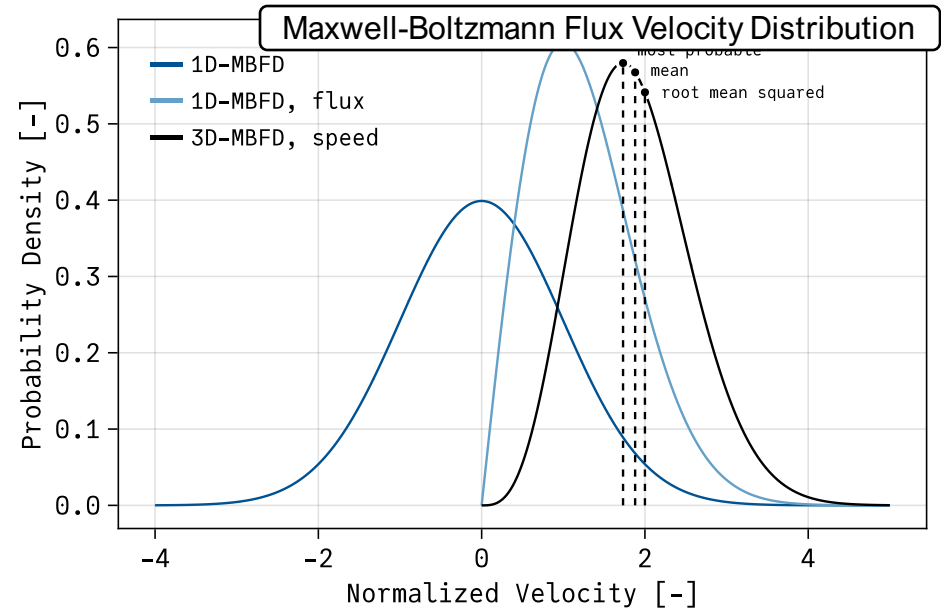
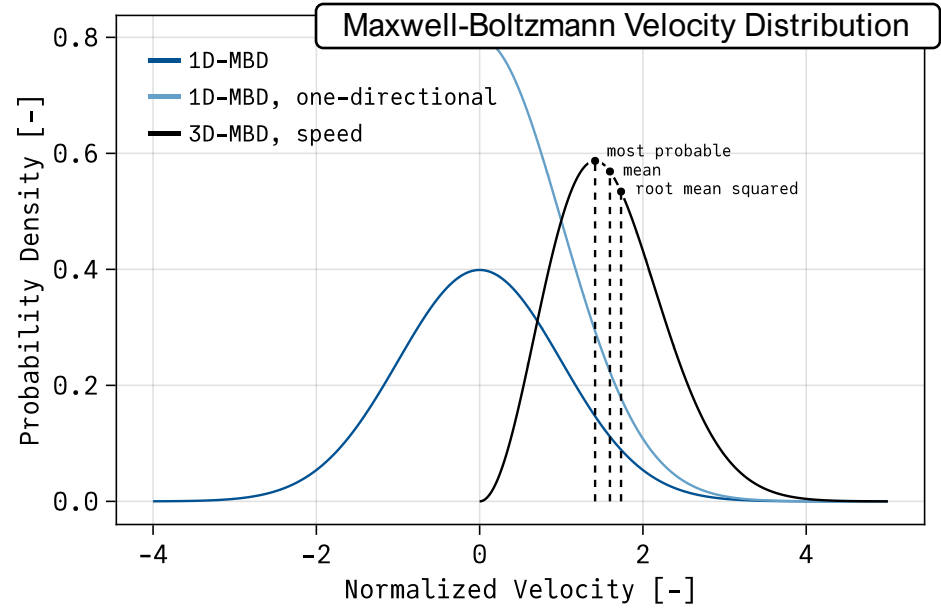


Simulation

Bounded



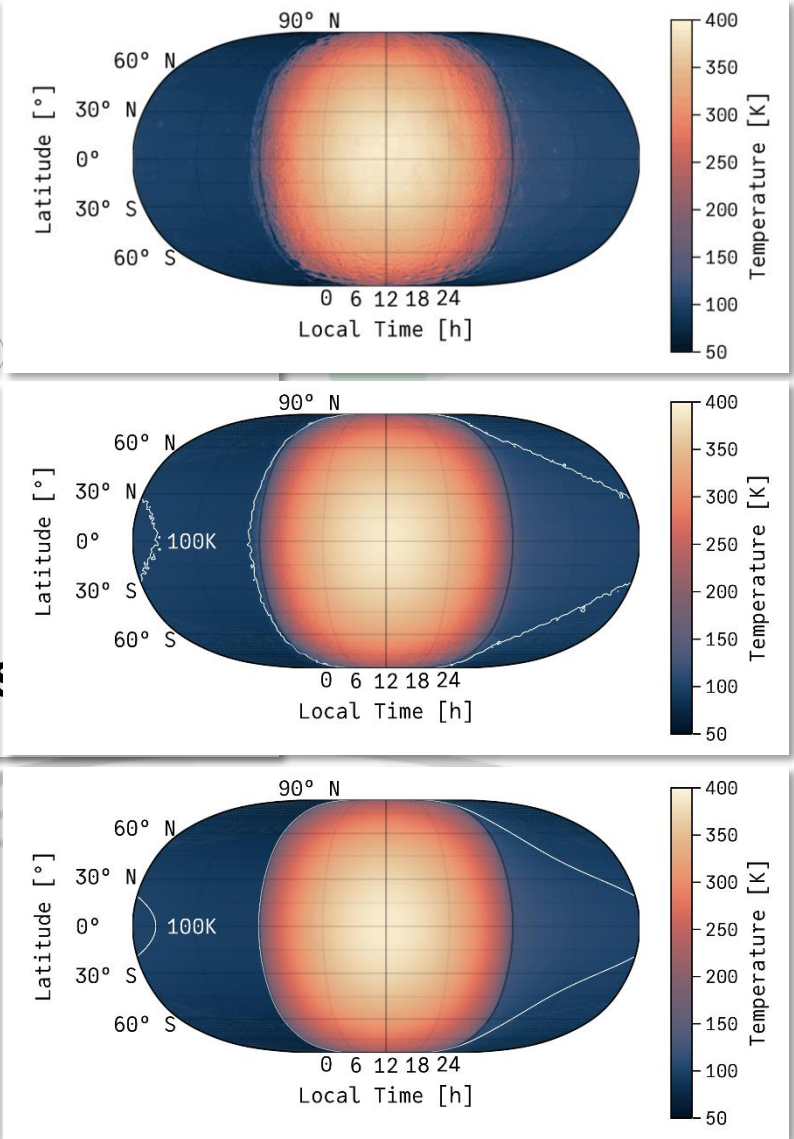
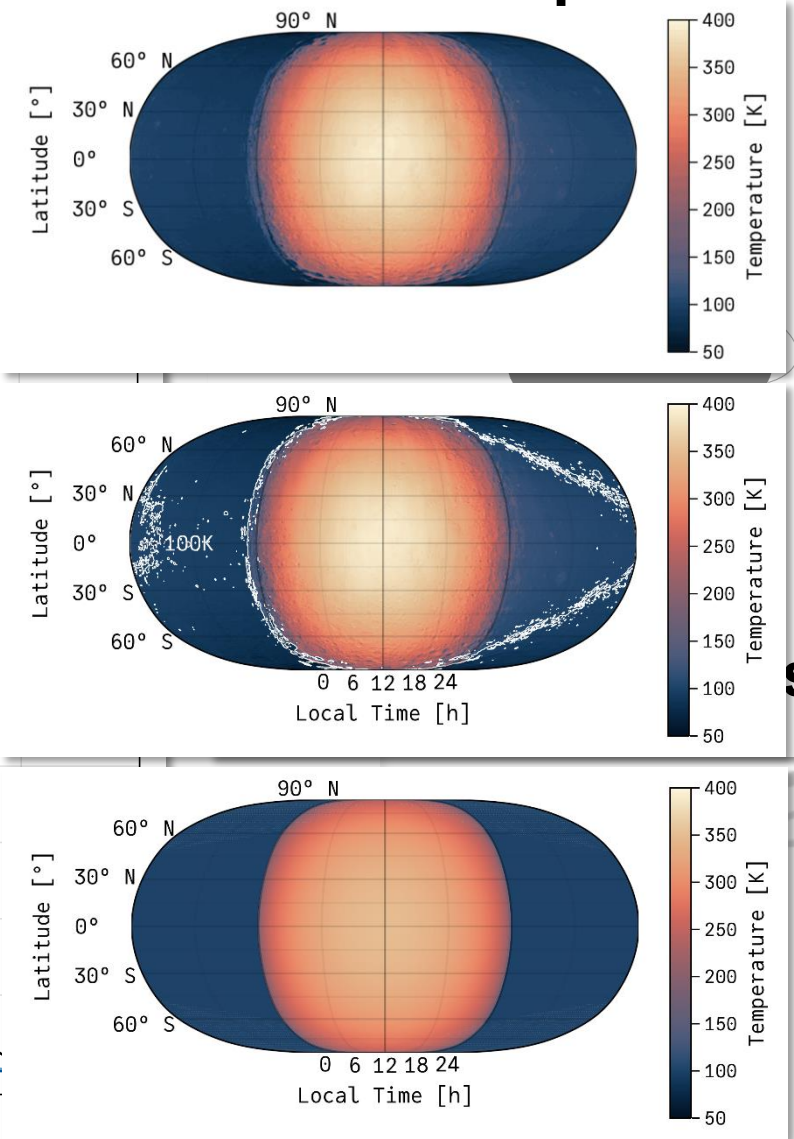
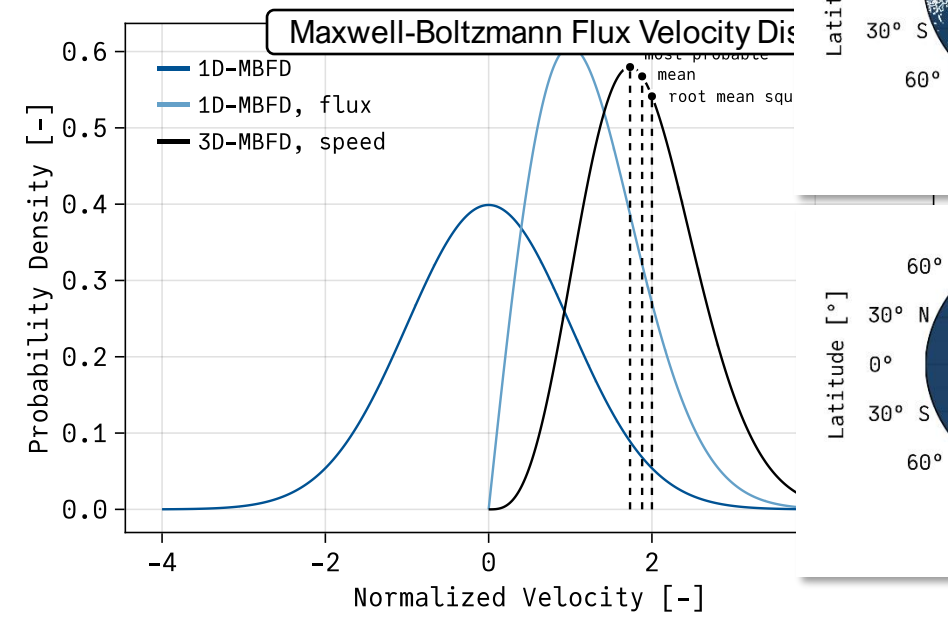
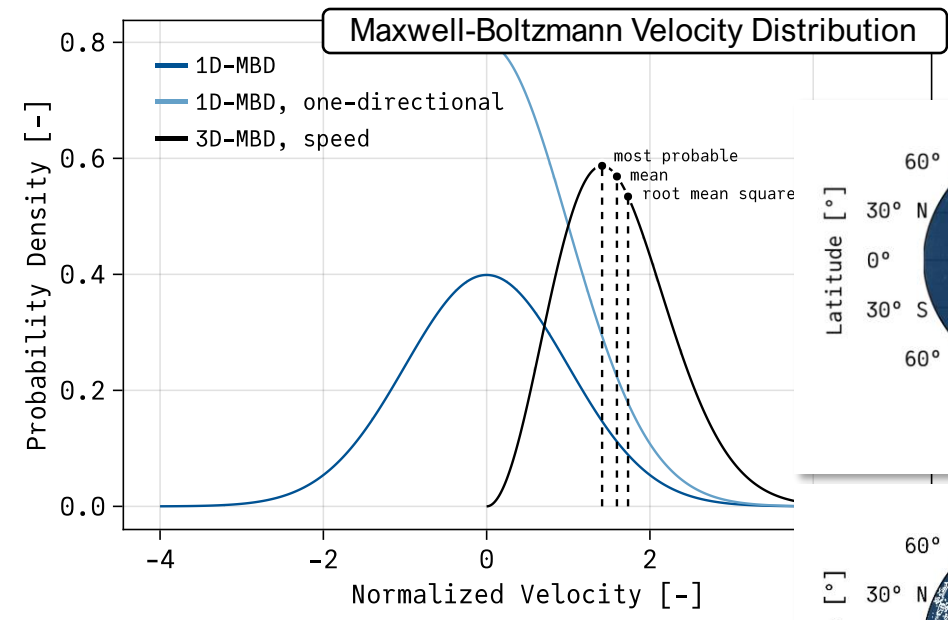
Velocity distributions



2D/3D Trajectories

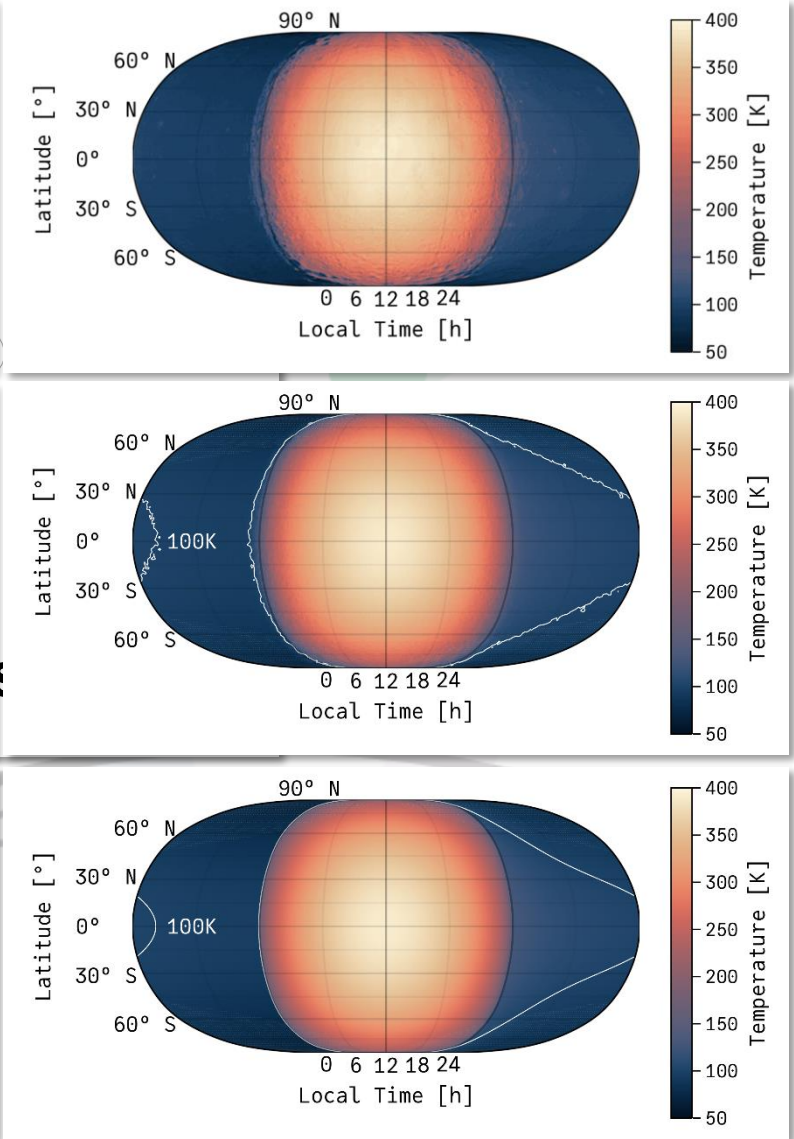
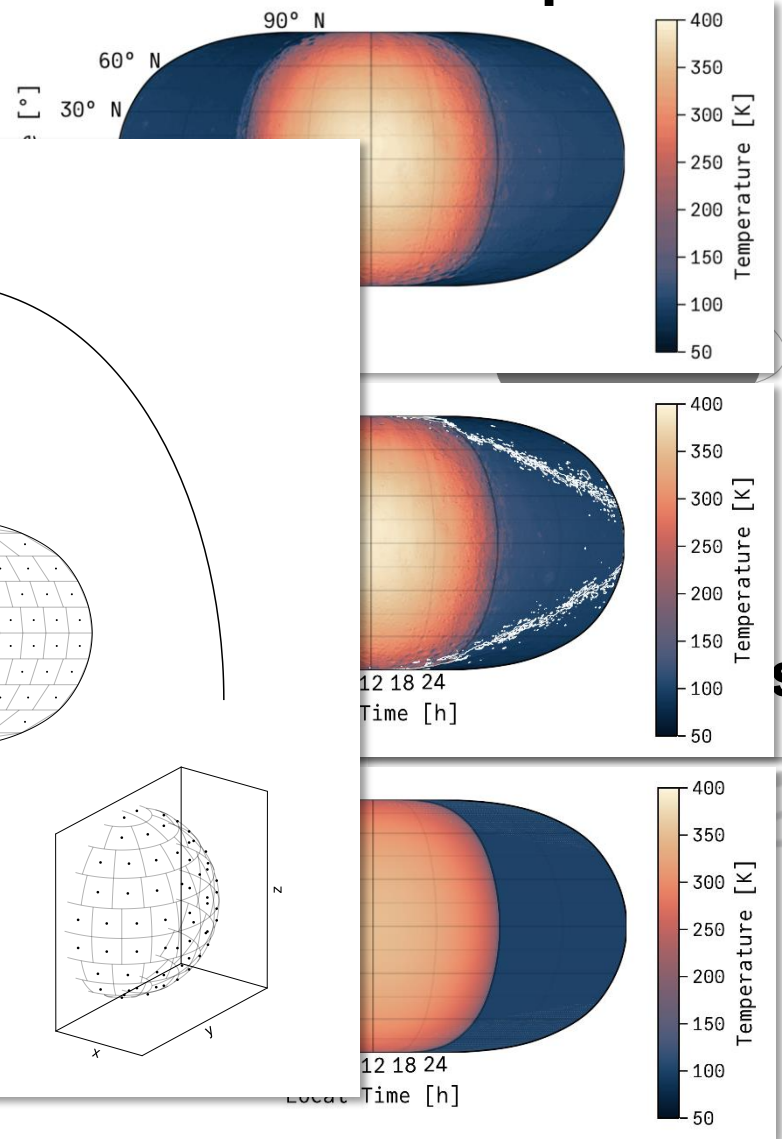
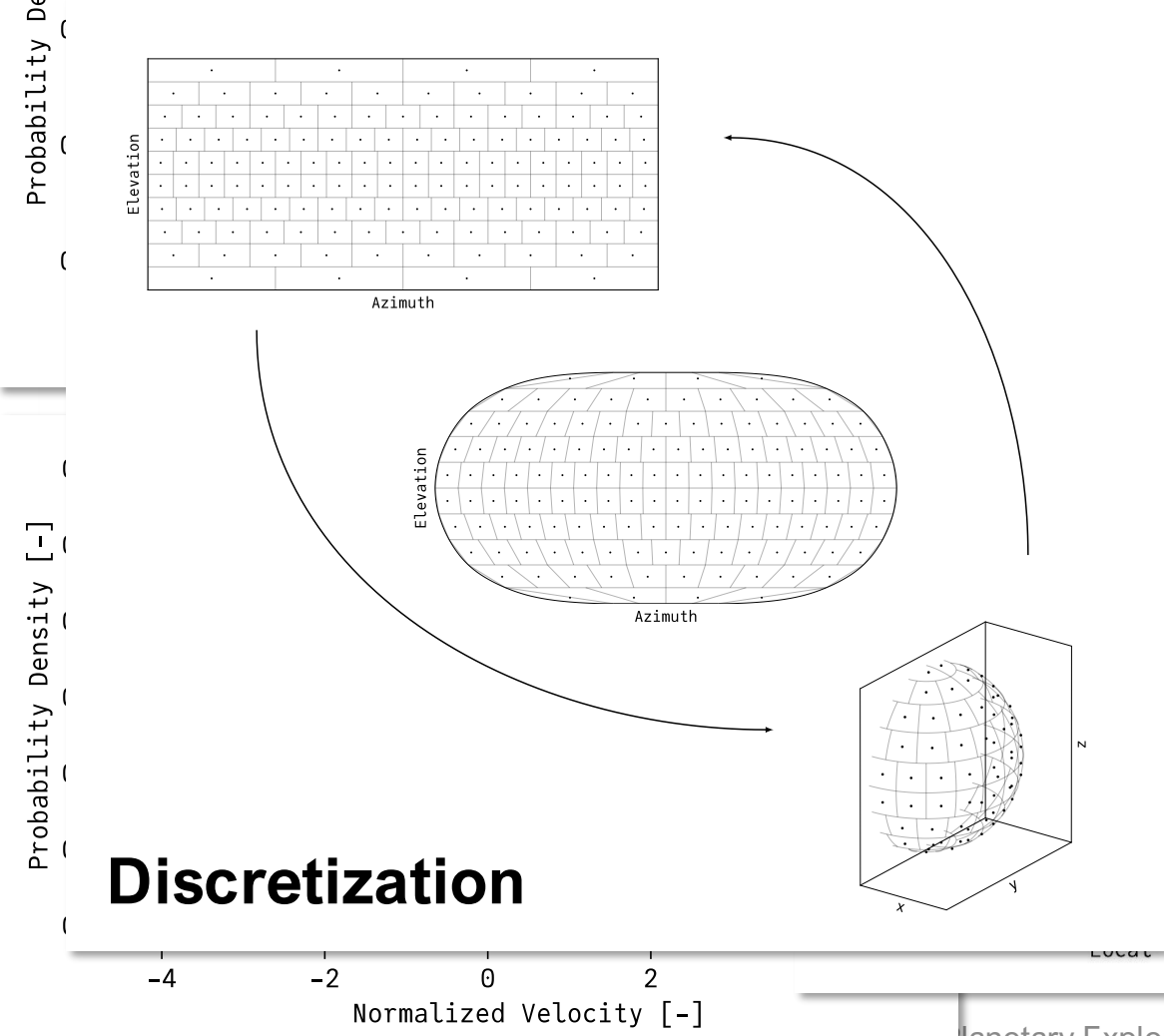
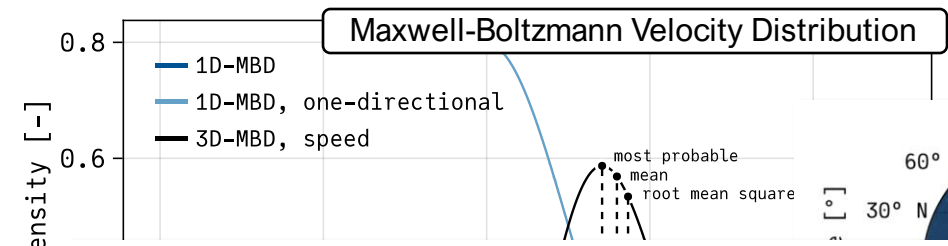
Velocity distributions

Temperature Distributions

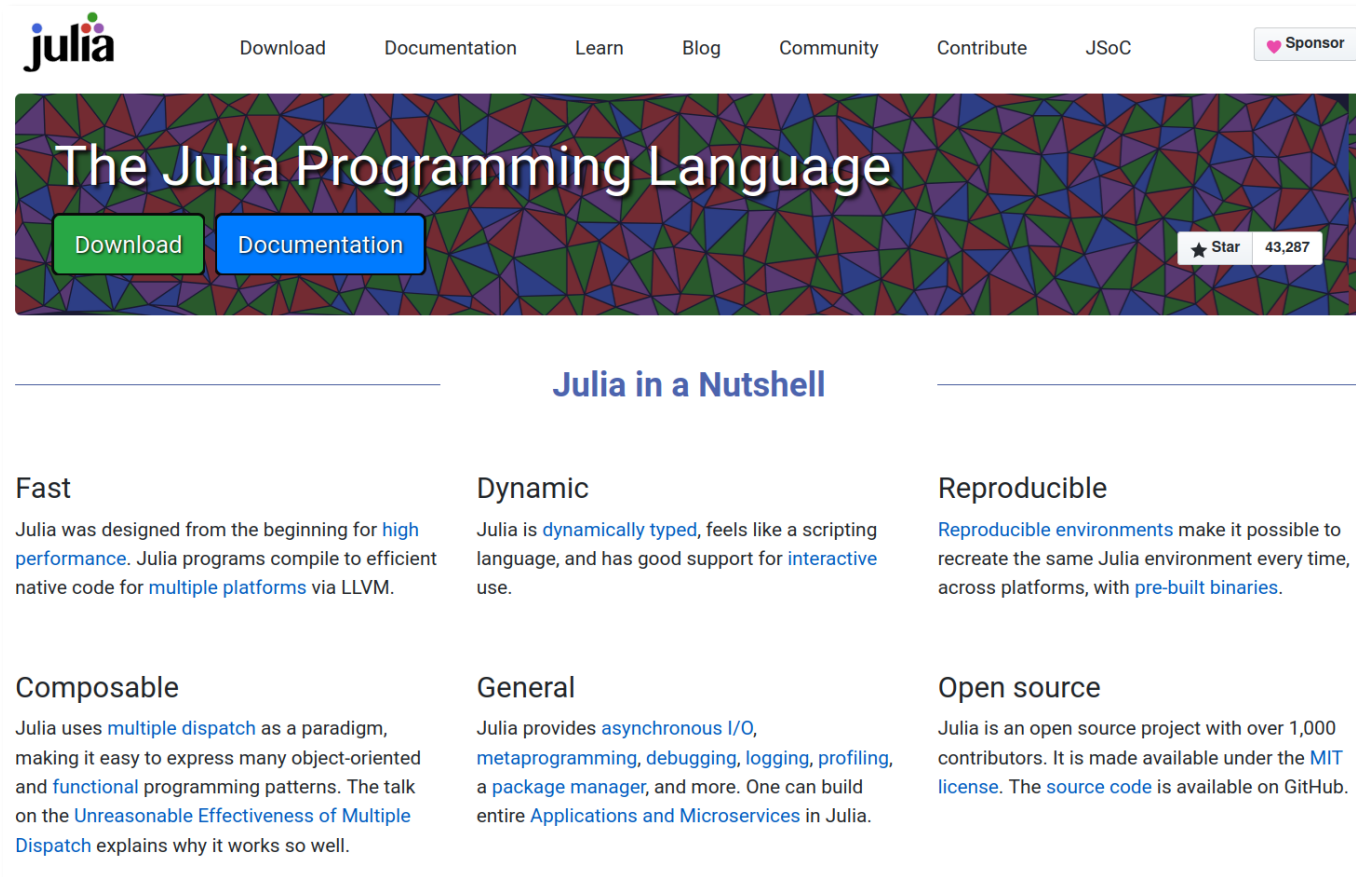


Velocity distributions

Temperature Distributions



Lunar Exosphere Simulation



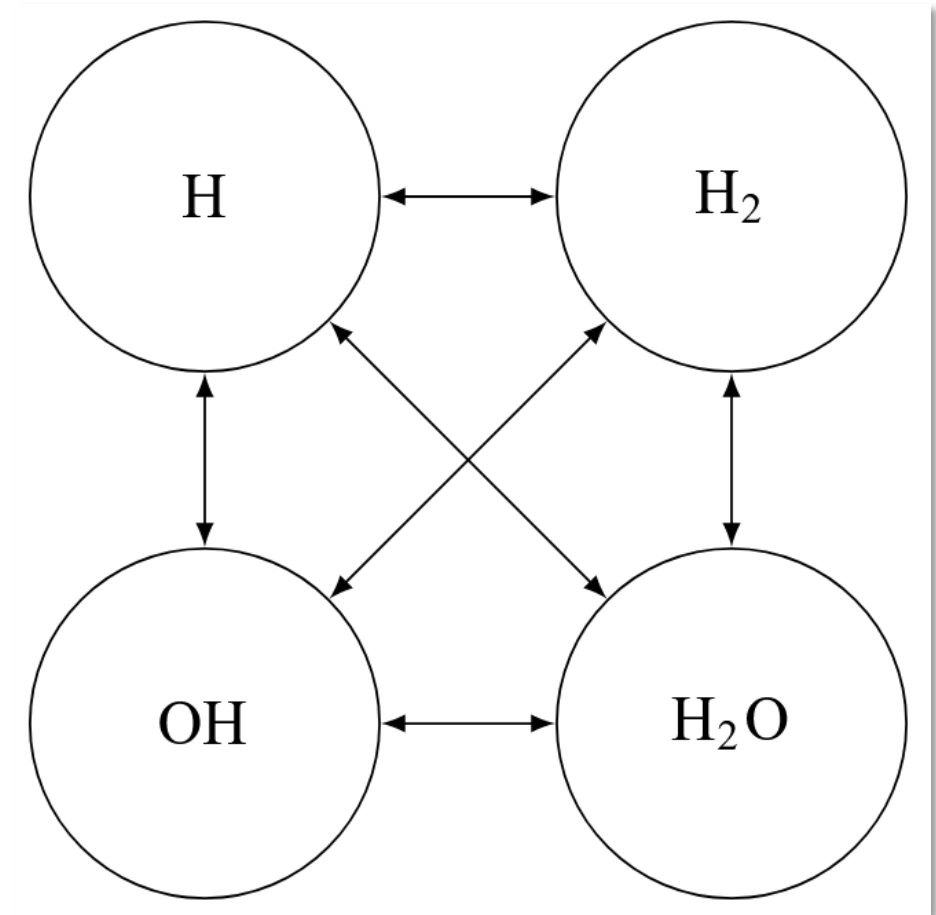
The screenshot shows the Julia Programming Language website. At the top, there is a navigation bar with links for Download, Documentation, Learn, Blog, Community, Contribute, JSoC, and a Sponsor button. Below the navigation bar is a large banner with a colorful geometric pattern. The banner contains the text "The Julia Programming Language" and two buttons: "Download" and "Documentation". To the right of the banner, there is a star icon and the number "43,287". Below the banner, the page is divided into three columns. The first column is titled "Julia in a Nutshell" and contains three sections: "Fast", "Dynamic", and "Reproducible". The second column contains two sections: "Composable" and "General". The third column contains one section: "Open source". Each section has a brief description of a feature of the Julia programming language.



<https://julialang.org/>

Lunar Water Exosphere Simulation

Conversion Reactions

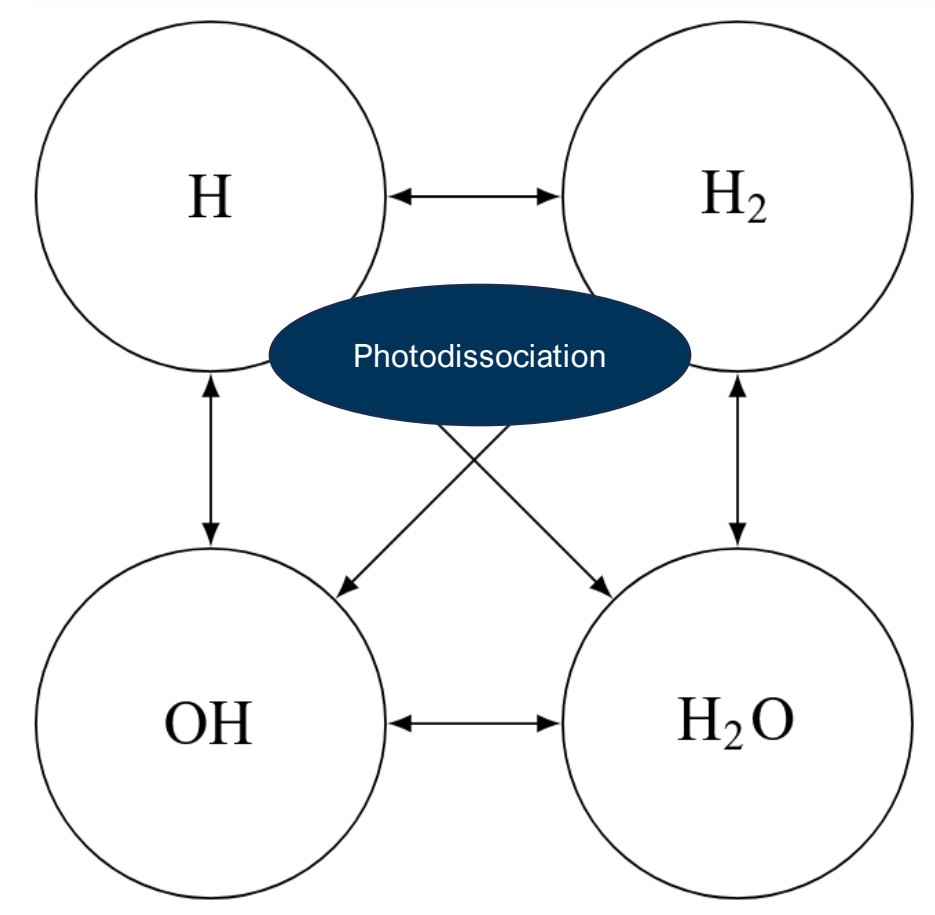


Lunar Water Exosphere Simulation

Conversion Reactions

Reaction	Quiet Sun Photoreaction Rate in 10^{-7} s^{-1}	Active Sun Photoreaction Rate in 10^{-7} s^{-1}
1 $\text{H} + \nu \rightarrow \text{H}^+ + \text{e}^-$	0.726	1.720
2 $\text{H}_2 + \nu \rightarrow \text{H}(1s) + \text{H}(1s)$	0.480	1.090
$\text{H}_2 + \nu \rightarrow \text{H}(1s) + \text{H}(2s \text{ or } 2p)$	0.344	0.821
$\text{H}_2 + \nu \rightarrow \text{H}_2^+ + \text{e}^-$	0.541	1.150
$\text{H}_2 + \nu \rightarrow \text{H} + \text{H}^+ + \text{e}^-$	0.095	0.279
17 $\text{OH} + \nu \rightarrow \text{O}(3p) + \text{H}$	(120.00) 65.400	(138.00) 71.700
$\text{OH} + \nu \rightarrow \text{O}(1d) + \text{H}$	(70.10) 6.350	(176.00) 15.100
$\text{OH} + \nu \rightarrow \text{O}(1s) + \text{H}$	(8.33) 0.671	(21.10) 1.640
$\text{OH} + \nu \rightarrow \text{OH}^+ + \text{e}^-$	(2.43) 2.470	(6.43) 6.520
18 $\text{H}_2\text{O} + \nu \rightarrow \text{OH} + \text{H}$	103.000	176.000
$\text{H}_2\text{O} + \nu \rightarrow \text{H}_2 + \text{O}(1d)$	5.970	14.800
$\text{H}_2\text{O} + \nu \rightarrow \text{H} + \text{H} + \text{O}$	7.550	19.100
$\text{H}_2\text{O} + \nu \rightarrow \text{H}_2\text{O}^+ + \text{e}^-$	3.310	8.280
$\text{H}_2\text{O} + \nu \rightarrow \text{H} + \text{OH}^+ + \text{e}^-$	0.554	1.510
$\text{H}_2\text{O} + \nu \rightarrow \text{H}_2 + \text{O}^+ + \text{e}^-$	0.059	0.221
$\text{H}_2\text{O} + \nu \rightarrow \text{OH} + \text{H}^+ + \text{e}^-$	0.131	0.407

Huebner et al., 1992



Lunar Water Exosphere Simulation

Conversion Reactions

Reaction	Quiet Sun Photoreaction Rate in 10^{-7} s^{-1}	Active Sun Photoreaction Rate in 10^{-7} s^{-1}
1 $\text{H} + \nu \rightarrow \text{H}^+ + \text{e}^-$	0.726	1.720
2 $\text{H}_2 + \nu \rightarrow \text{H}(1s) + \text{H}(1s)$	0.480	1.090
$\text{H}_2 + \nu \rightarrow \text{H}(1s) + \text{H}(2s \text{ or } 2p)$	0.344	0.821
$\text{H}_2 + \nu \rightarrow \text{H}_2^+ + \text{e}^-$	0.541	1.150
$\text{H}_2 + \nu \rightarrow \text{H} + \text{H}^+ + \text{e}^-$	0.095	0.279
17 $\text{OH} + \nu \rightarrow \text{O}(3p) + \text{H}$	(120.00) 65.400	(138.00) 71.700
$\text{OH} + \nu \rightarrow \text{O}(1d) + \text{H}$	(70.10) 6.350	(176.00) 15.100
$\text{OH} + \nu \rightarrow \text{O}(1s) + \text{H}$	(8.33) 0.671	(21.10) 1.640
$\text{OH} + \nu \rightarrow \text{OH}^+ + \text{e}^-$	(2.43) 2.470	(6.43) 6.520
18 $\text{H}_2\text{O} + \nu \rightarrow \text{OH} + \text{H}$	103.000	176.000

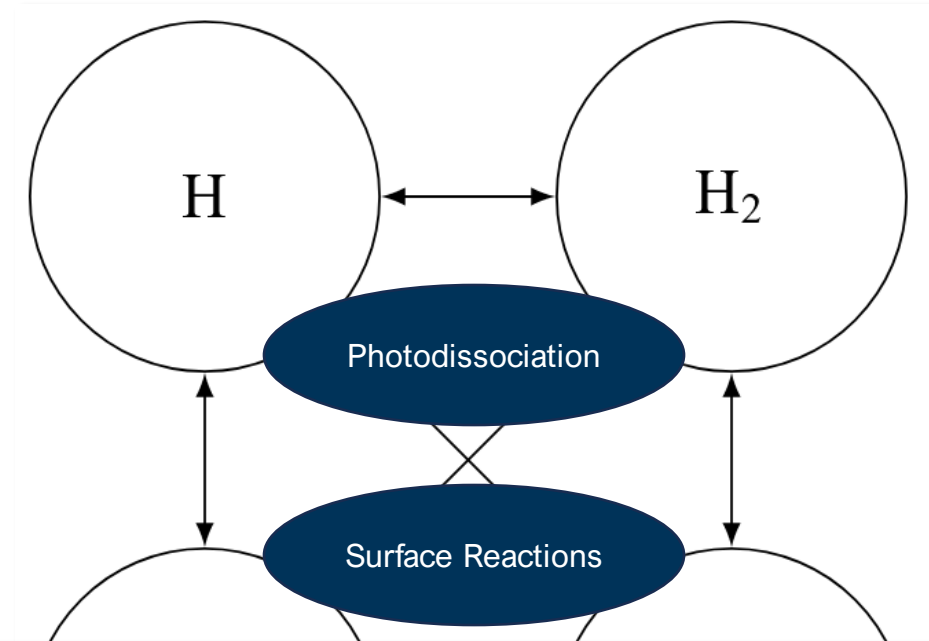
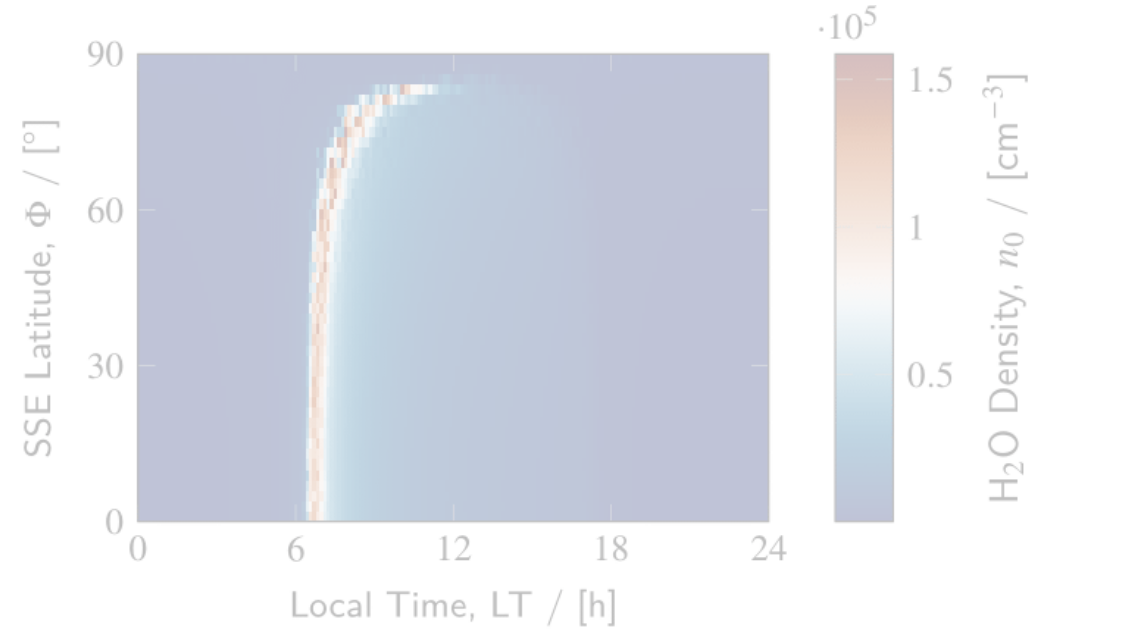
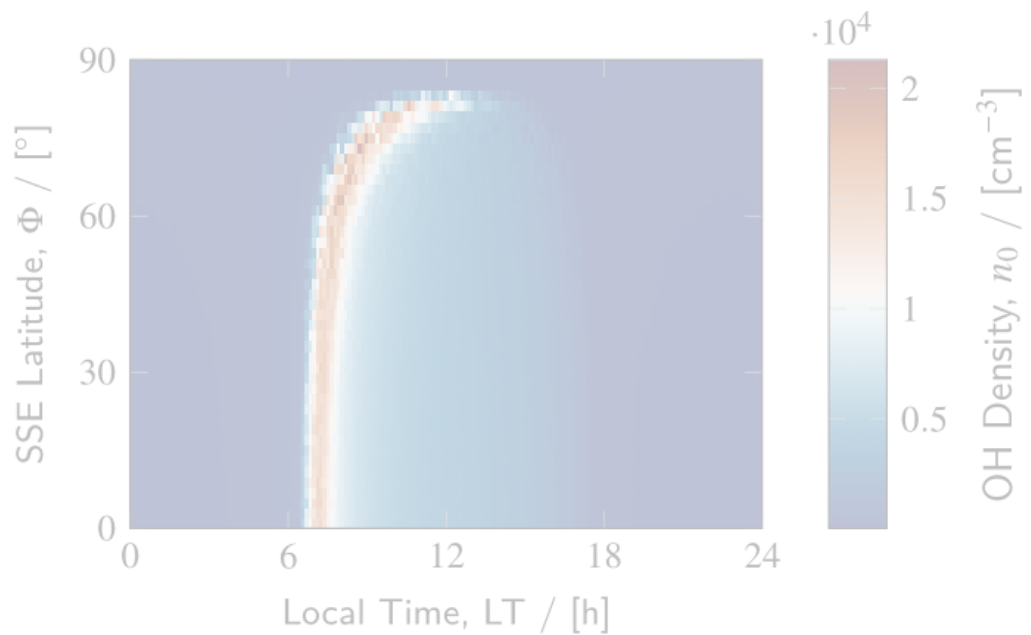
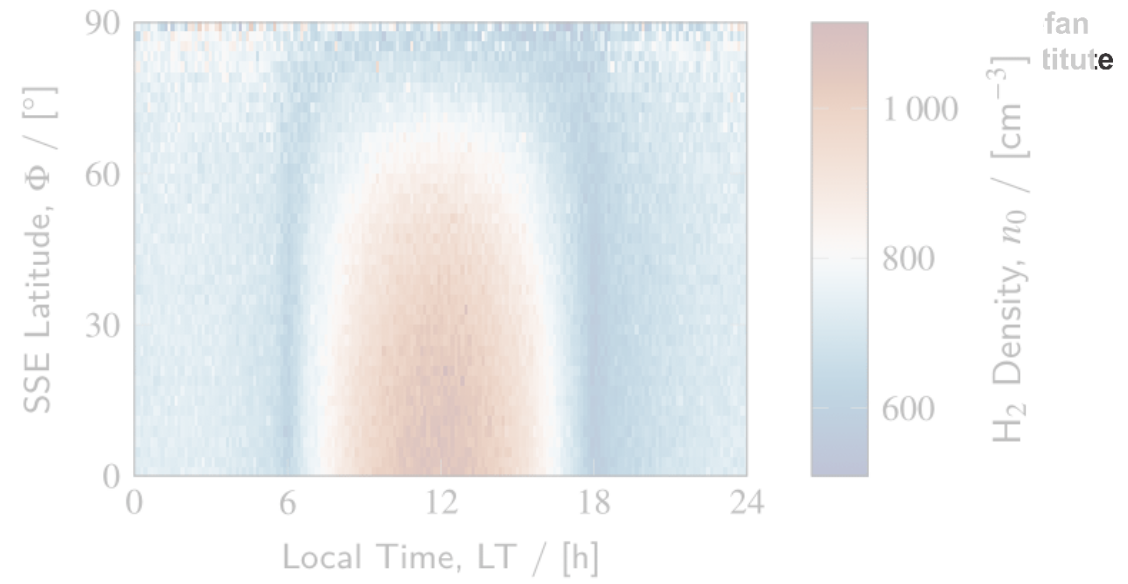
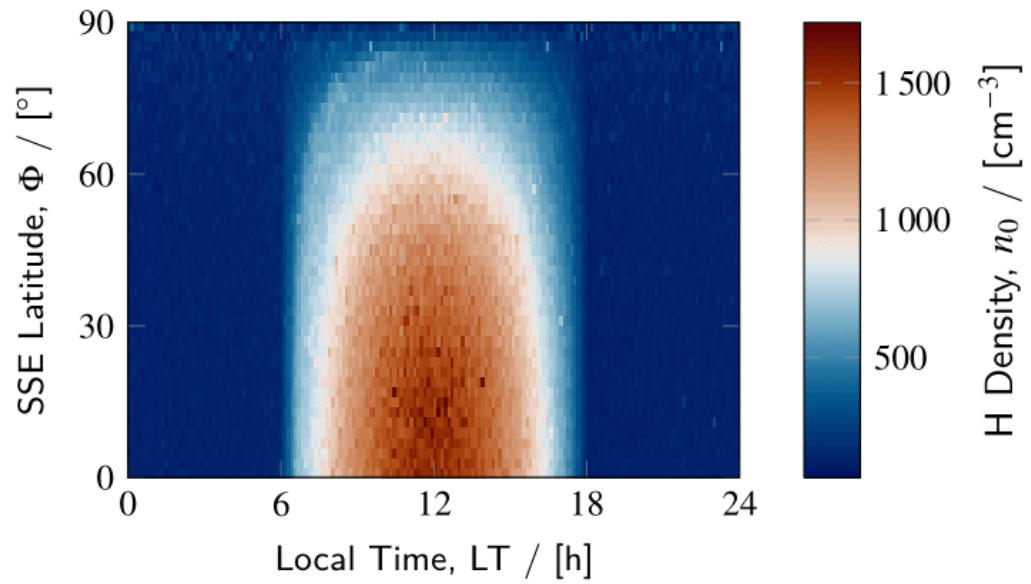
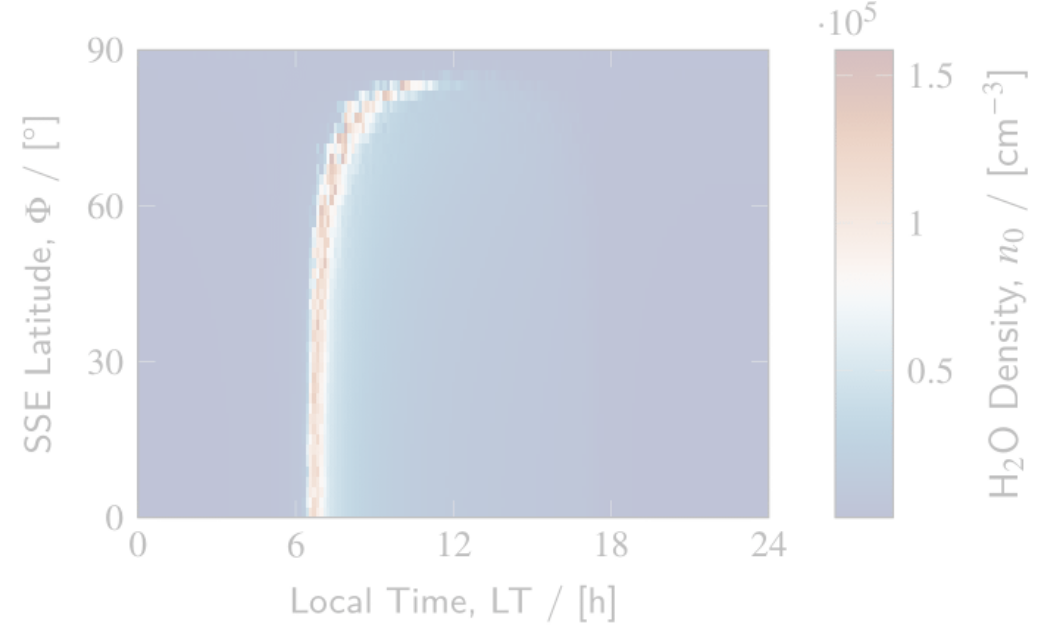
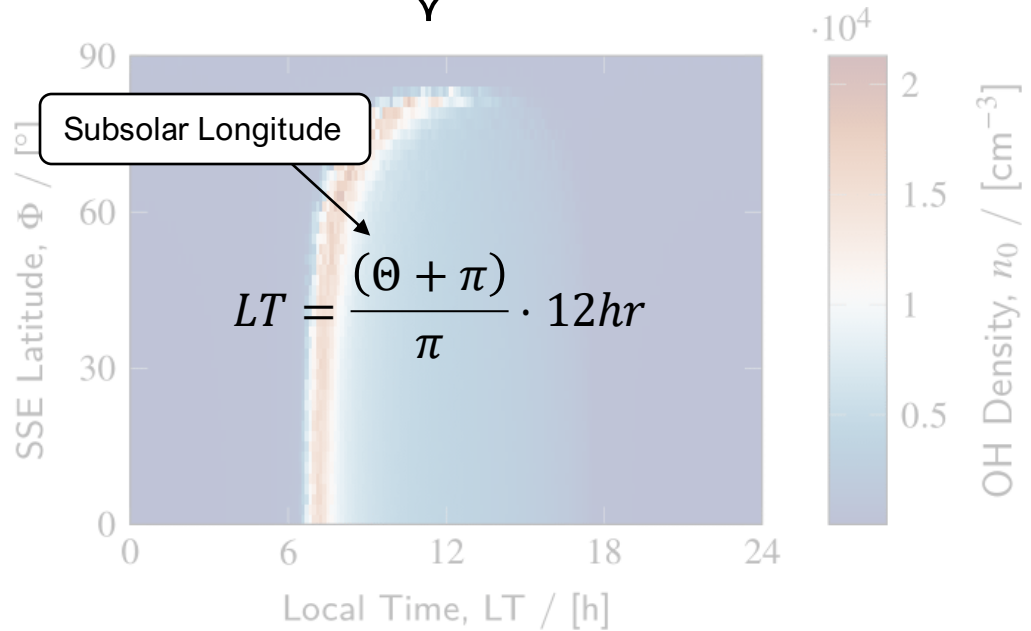
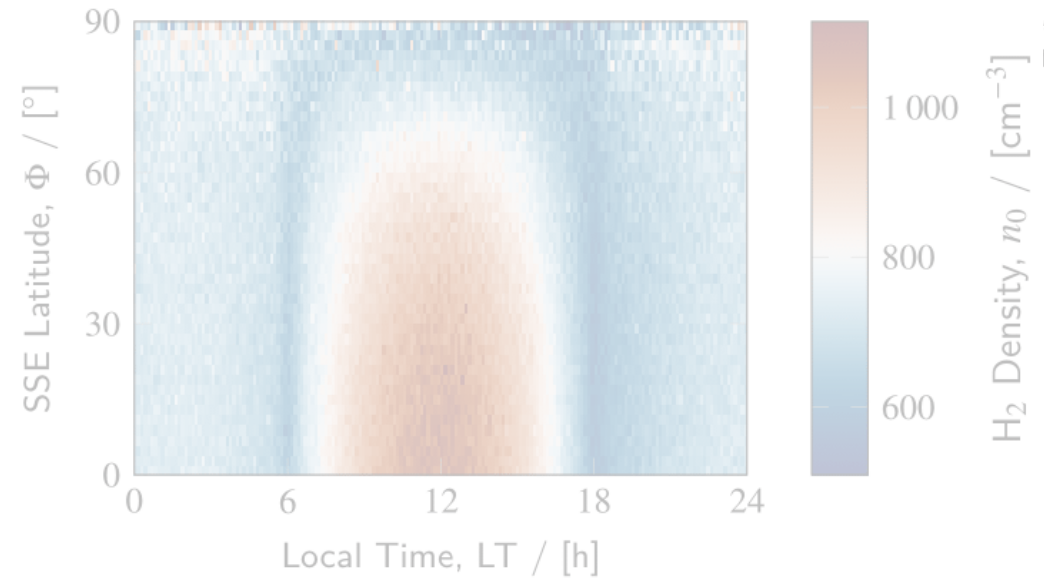
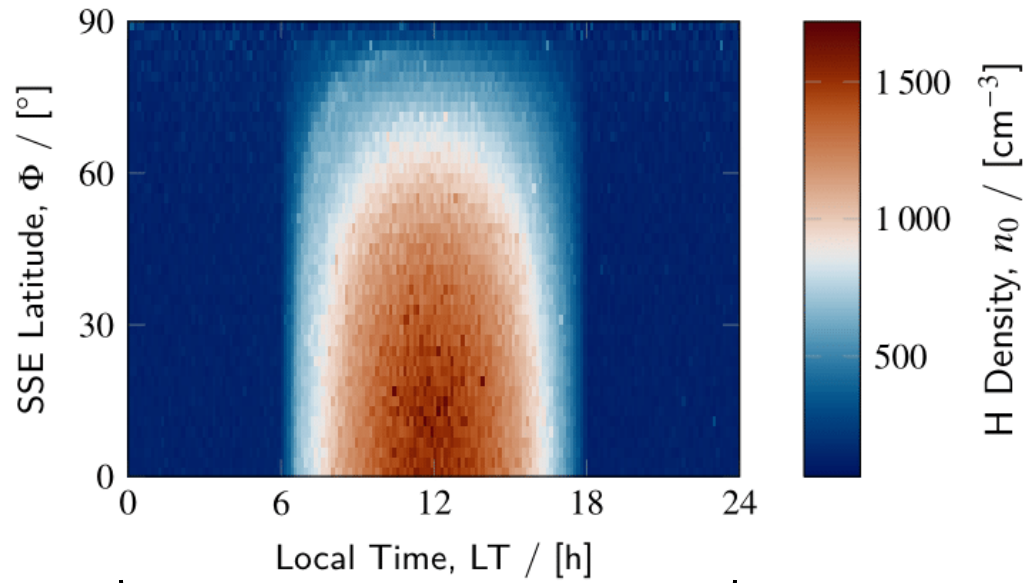


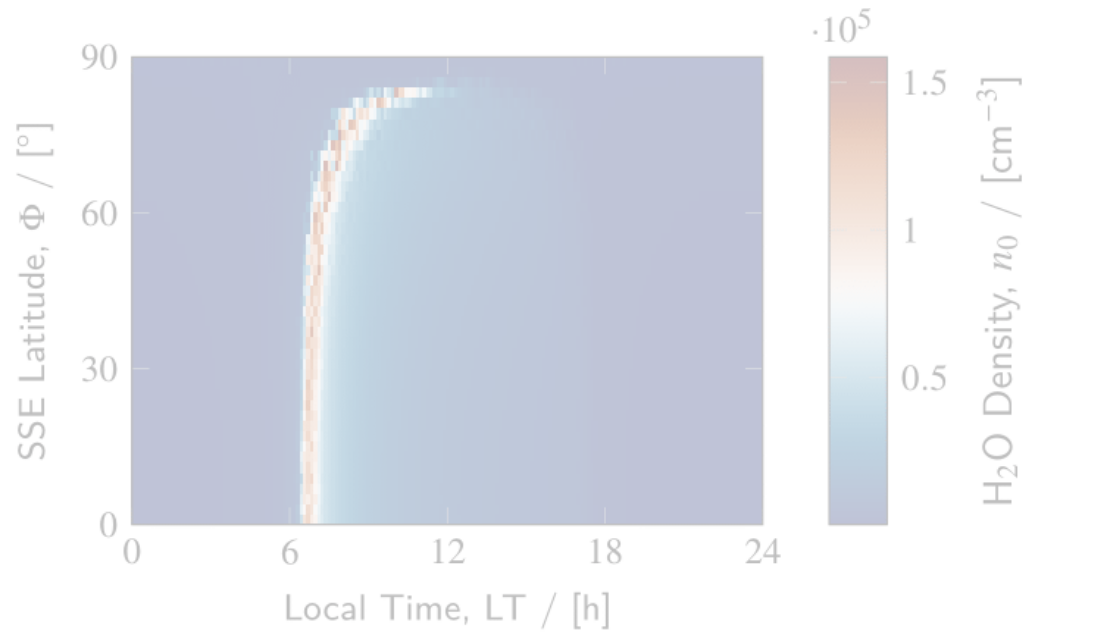
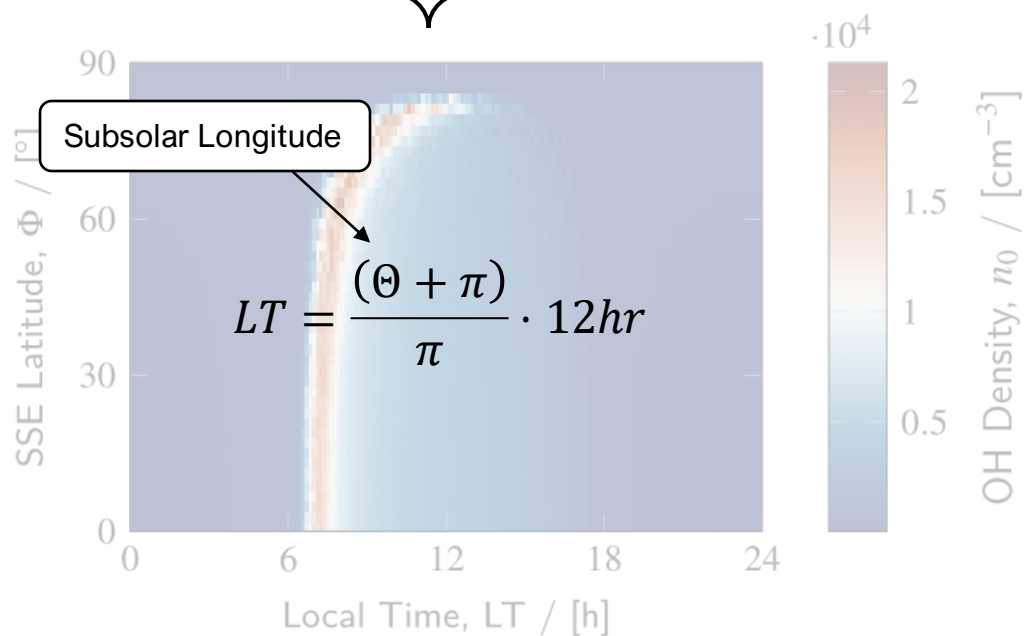
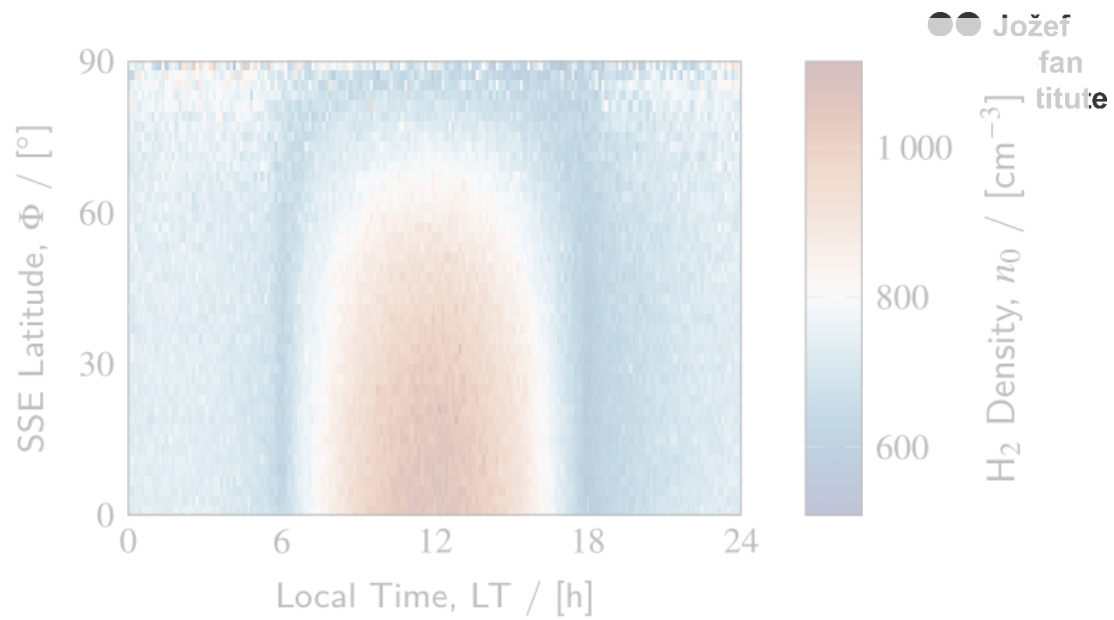
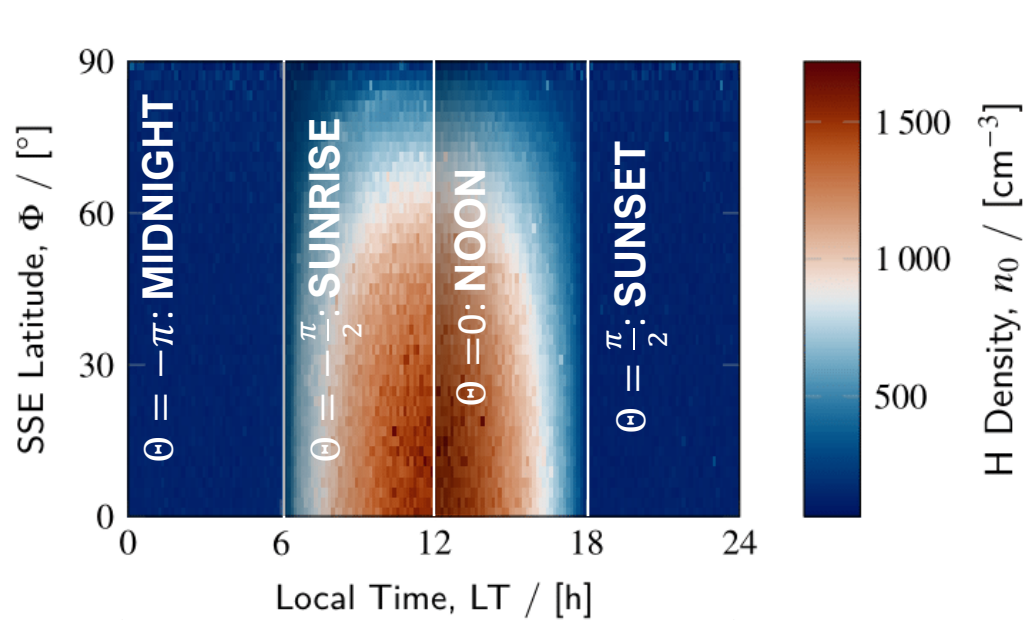
Table 1. Fractions of Incident Protons Entering Each Branch After Surface Interaction

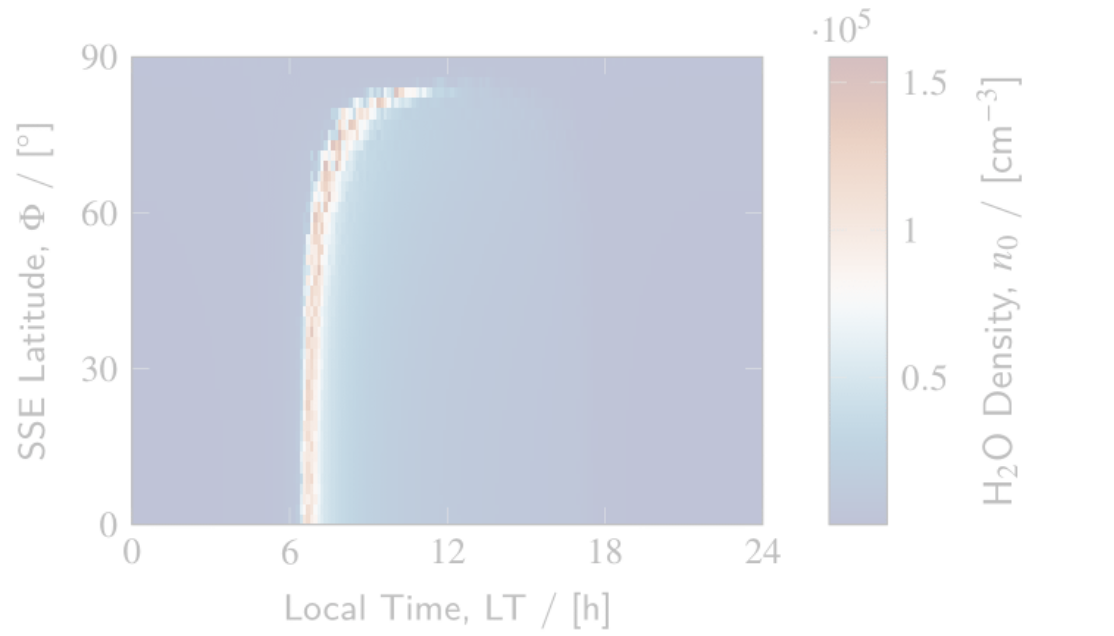
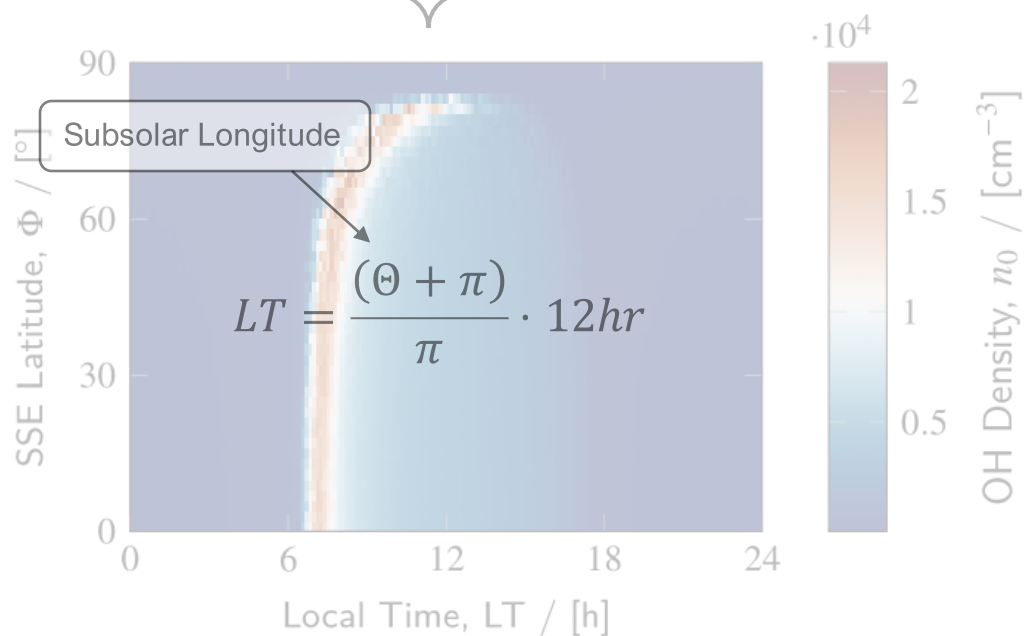
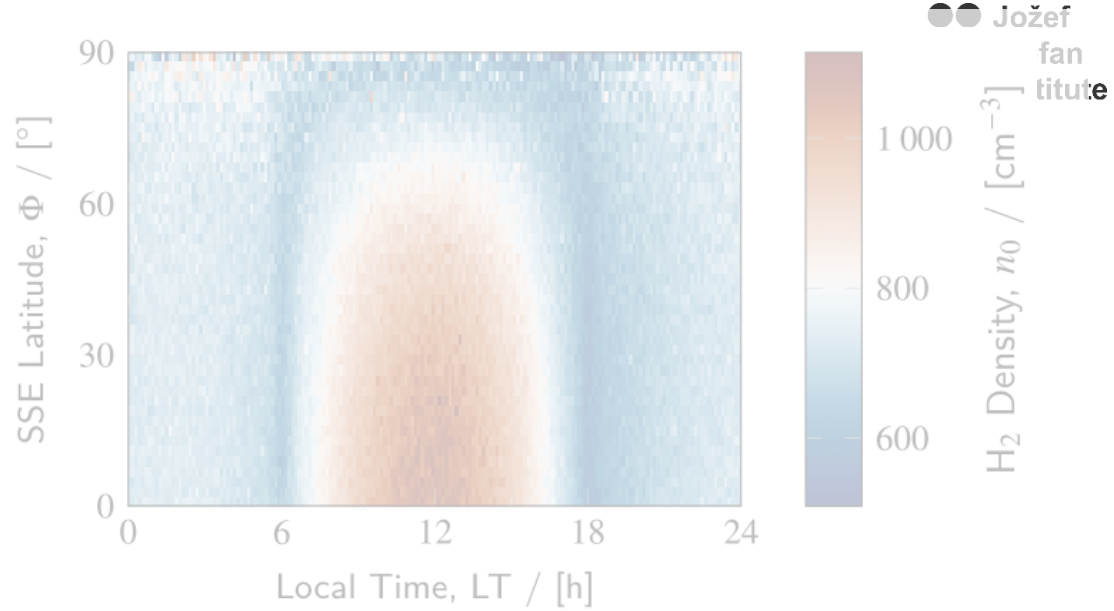
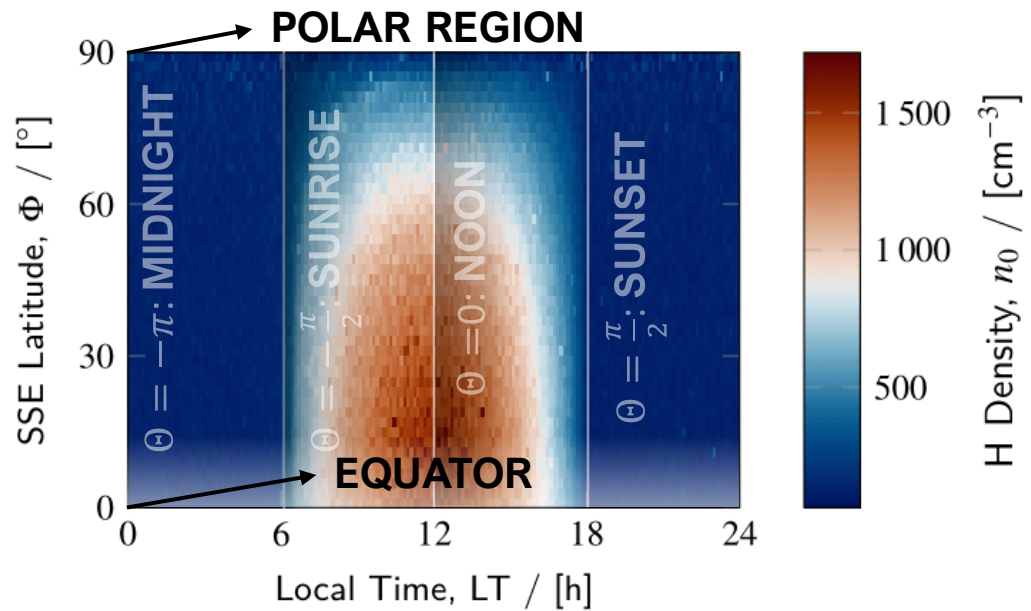
Backscatter H	Sputtered H	Desorbing H	Convert to H_2	Convert to OH	Convert to H_2O
.01	.0001	.27	.6	.1	.02

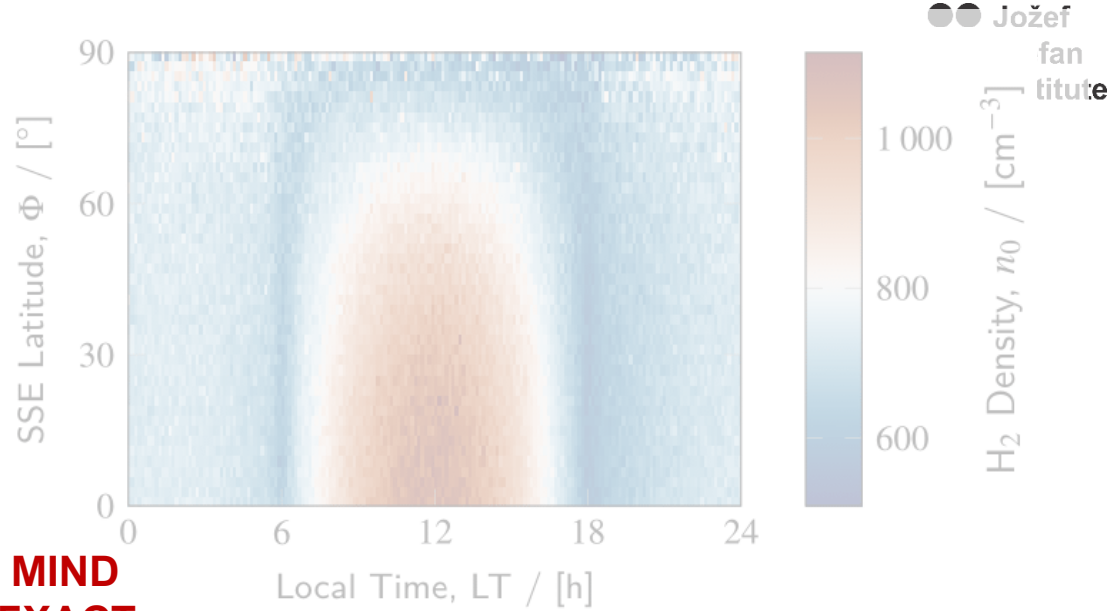
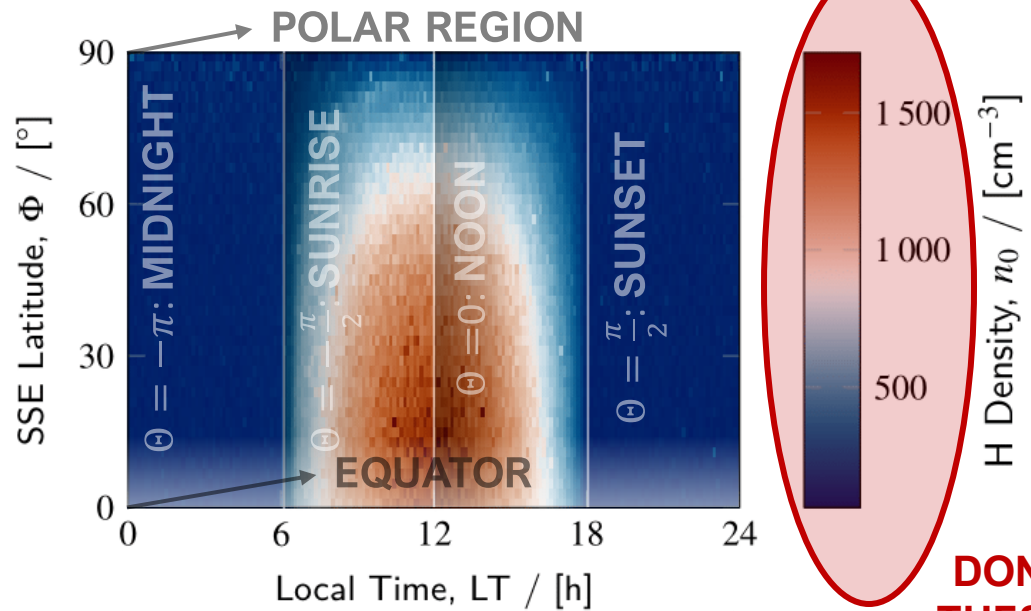
Crider and Vondrak, 2002



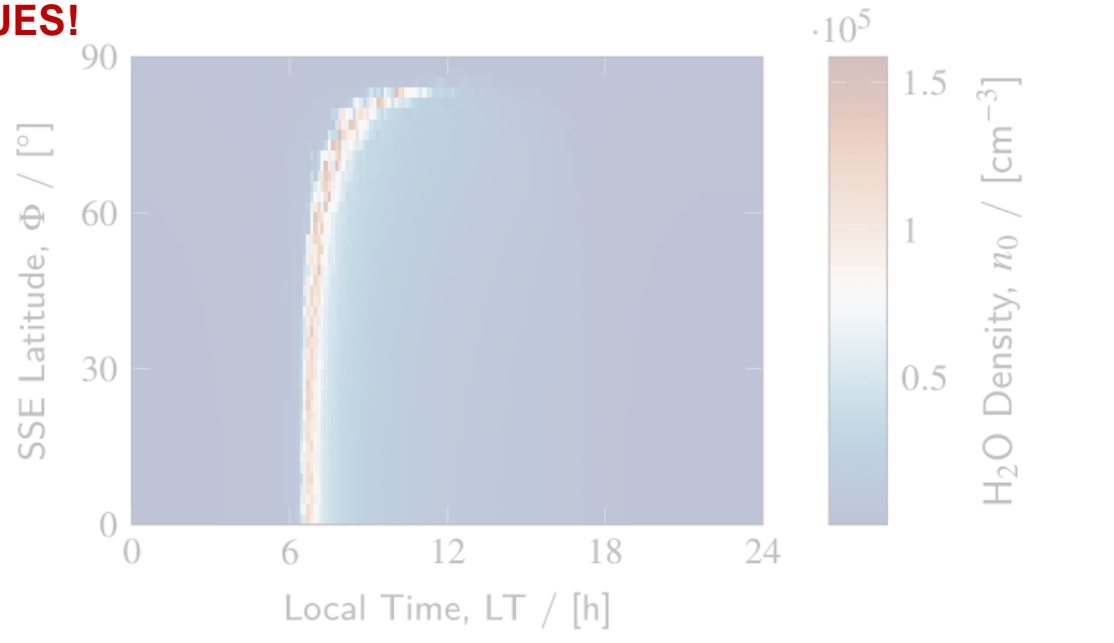
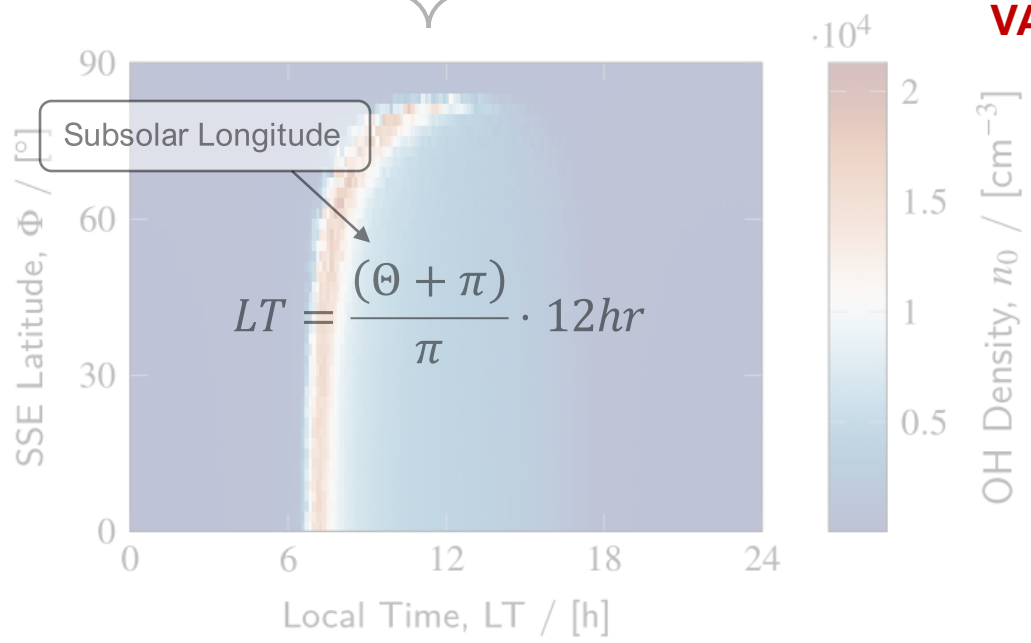


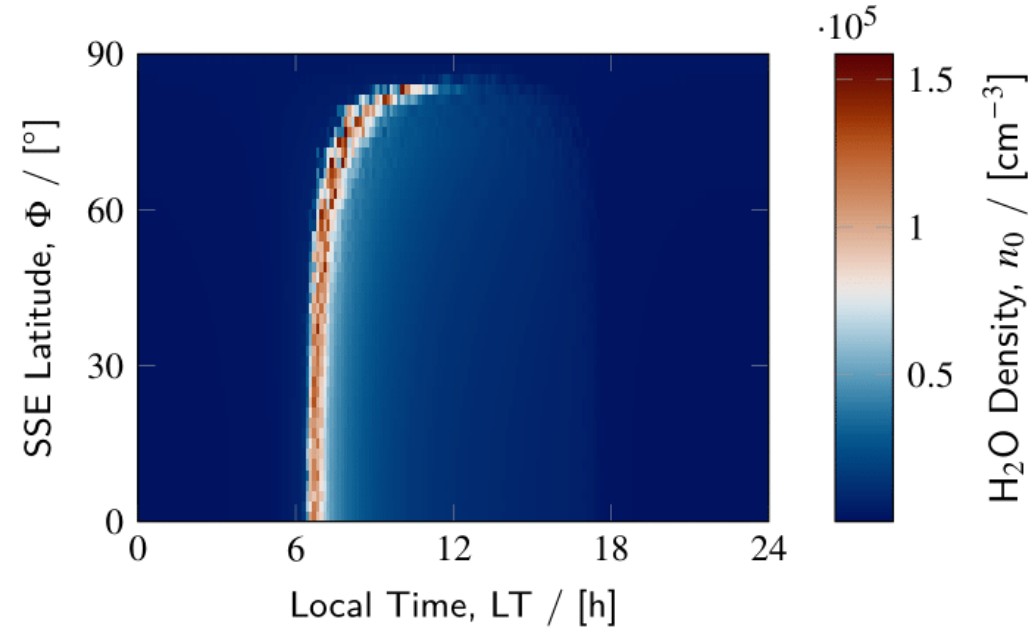
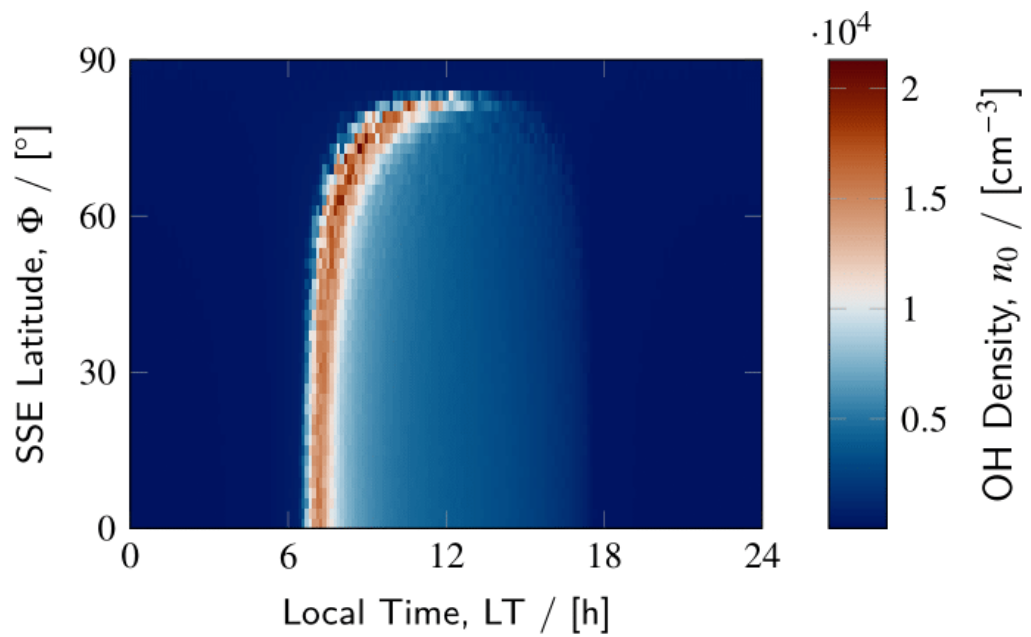
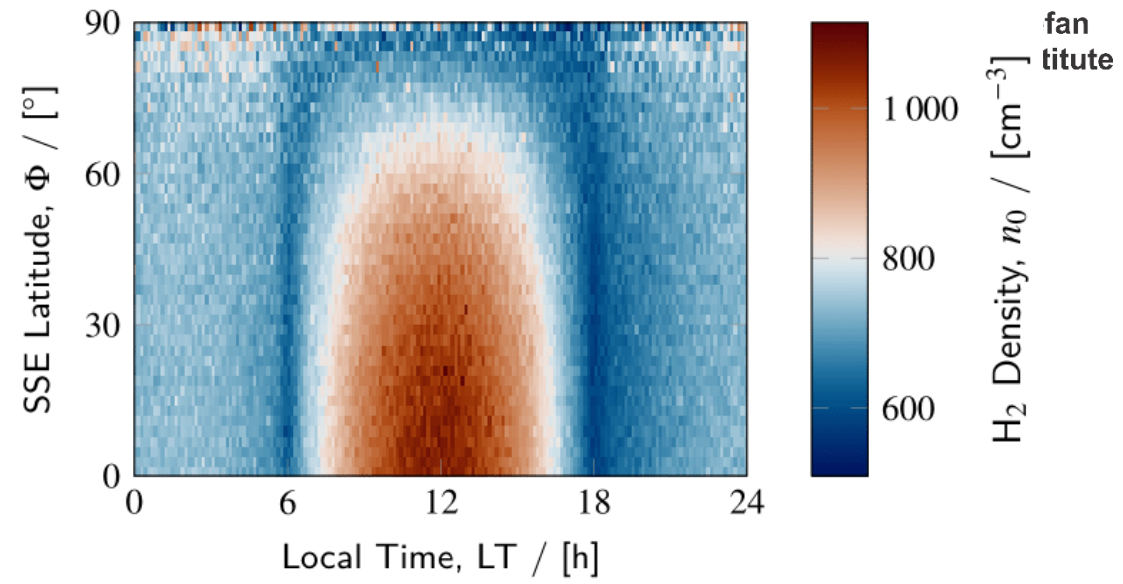
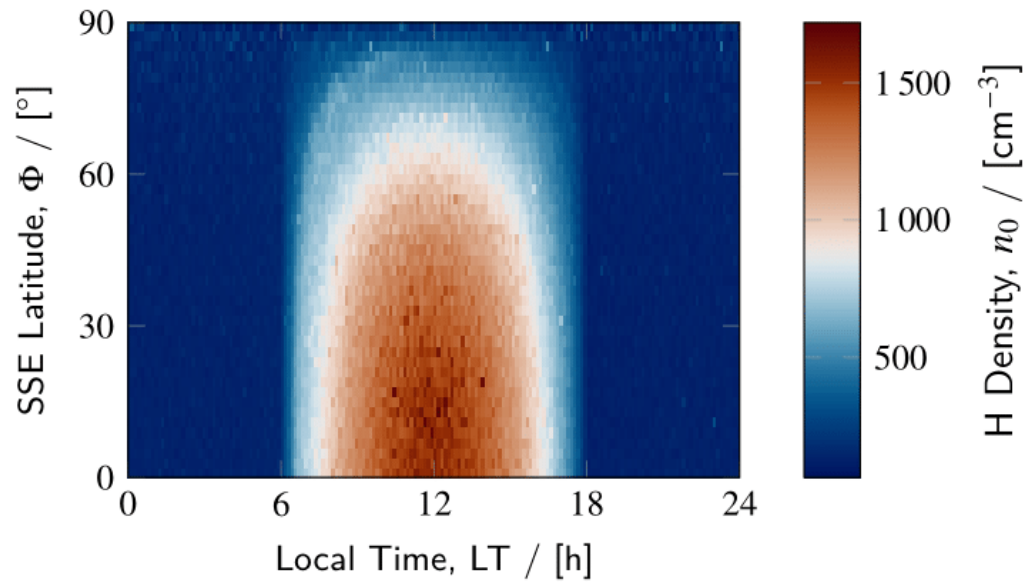


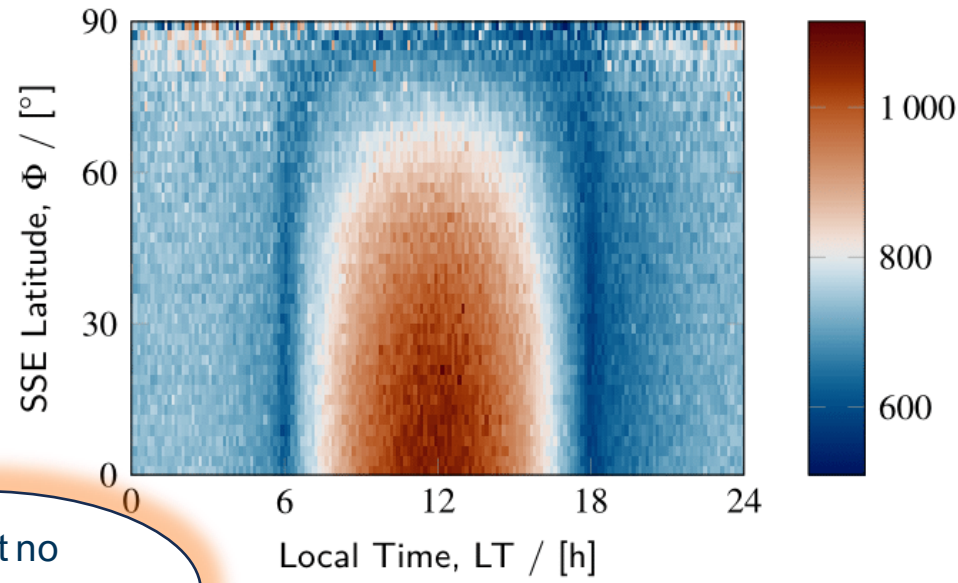
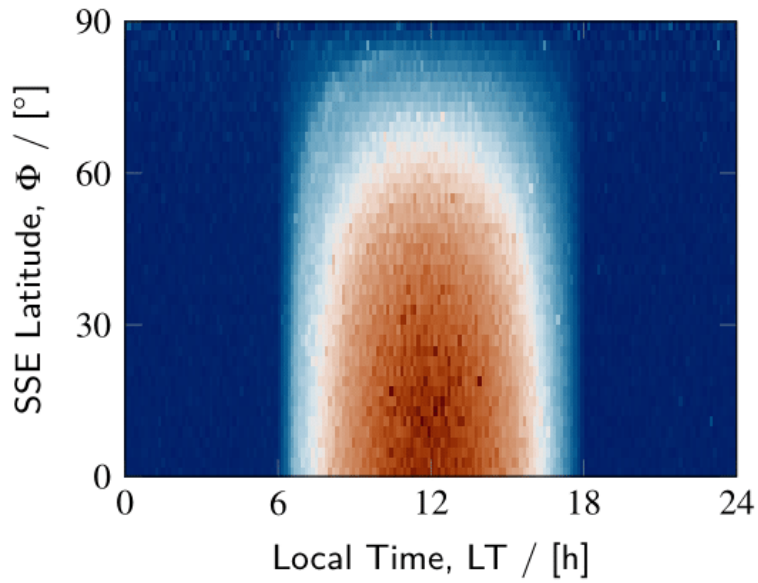




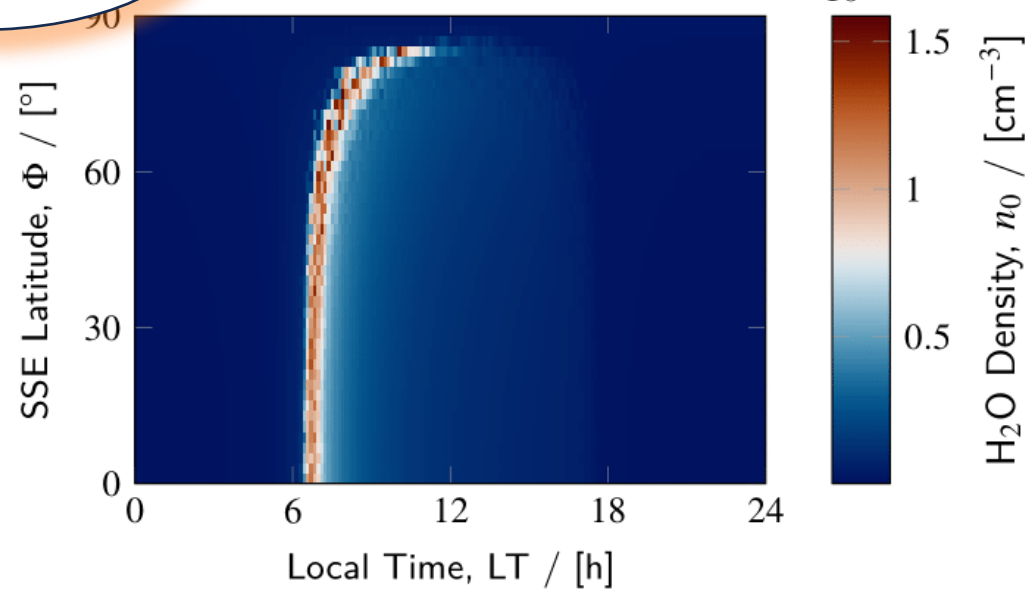
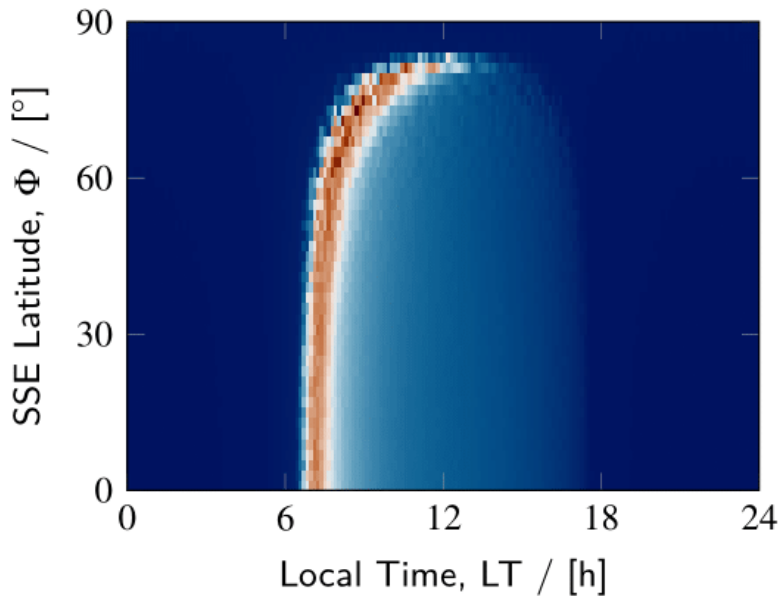
DON'T MIND THESE EXACT VALUES!

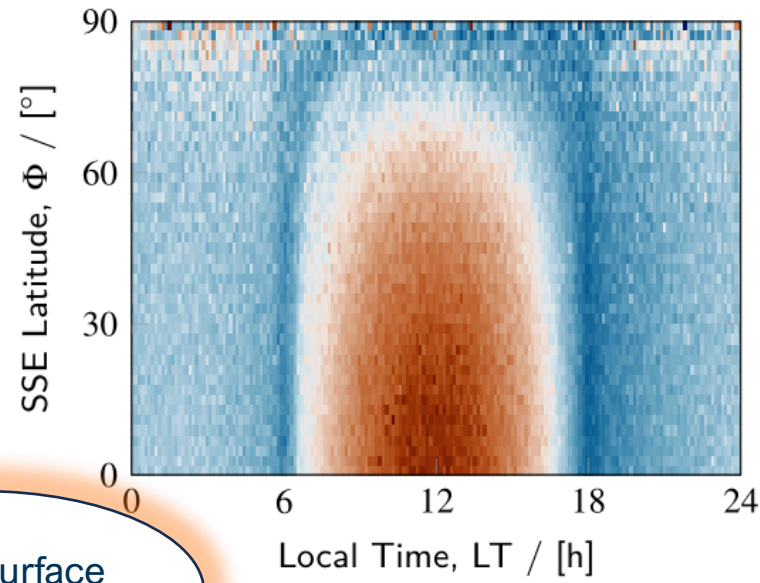
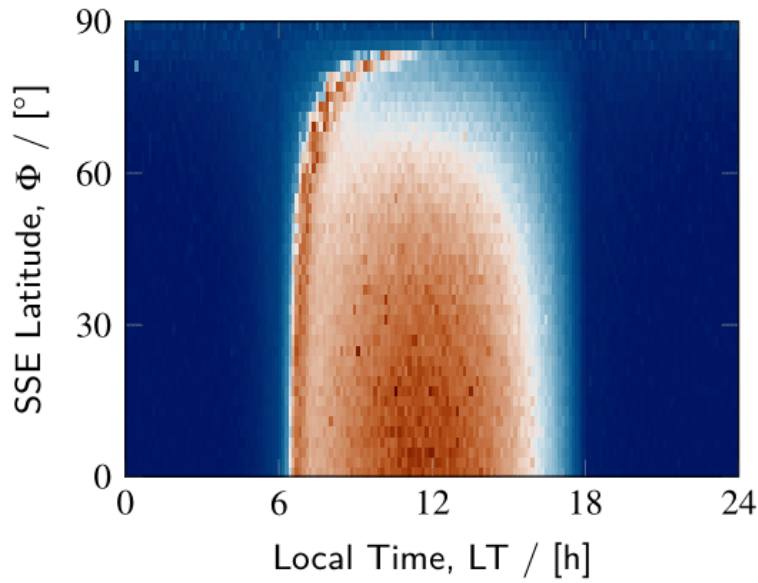




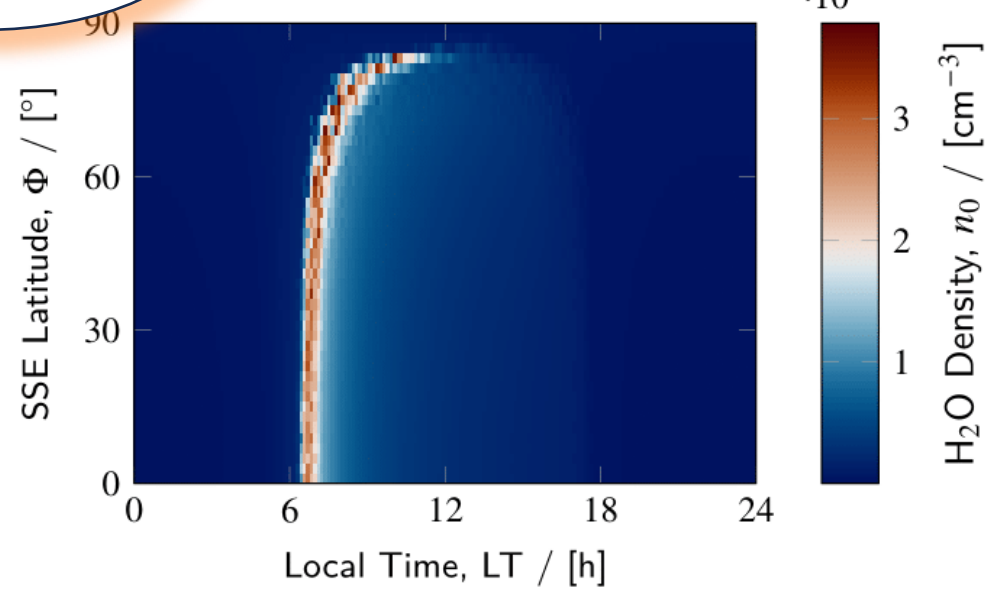
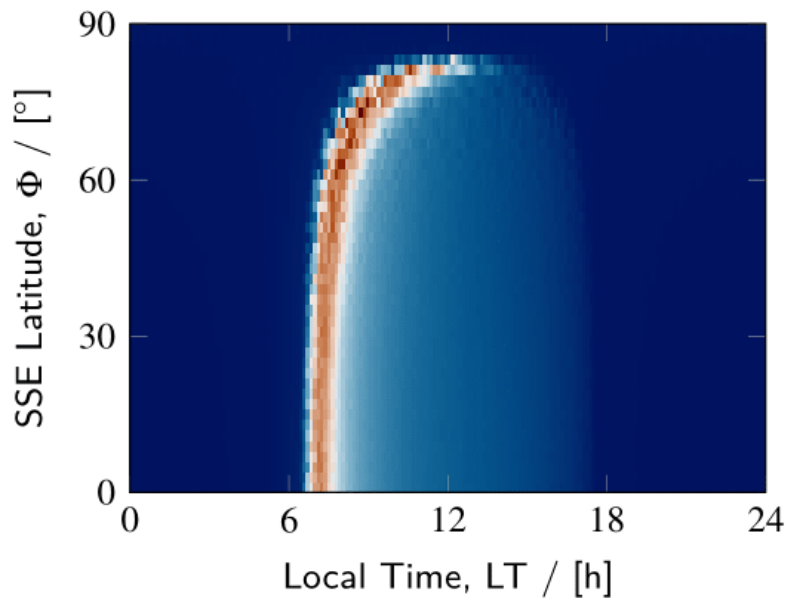


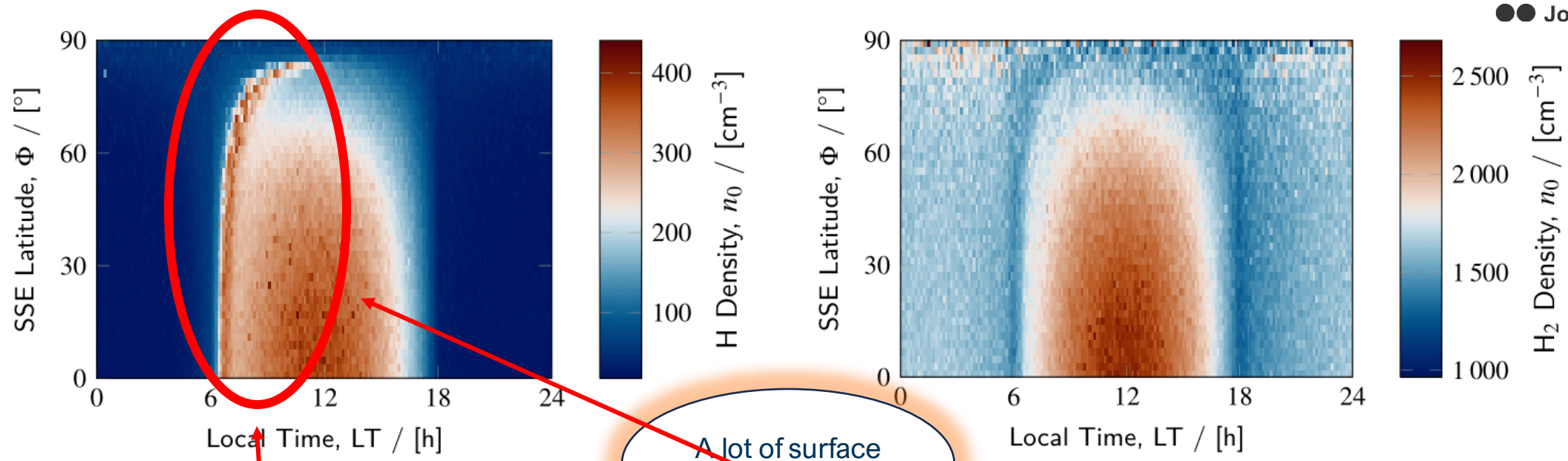
Almost no
surface
reactivity



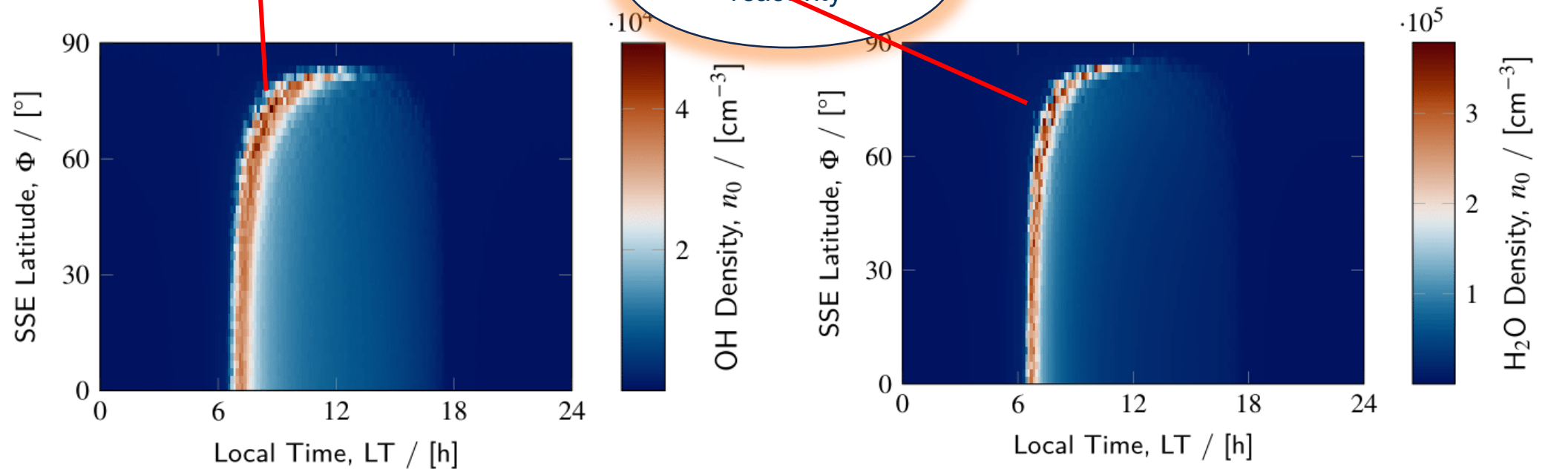


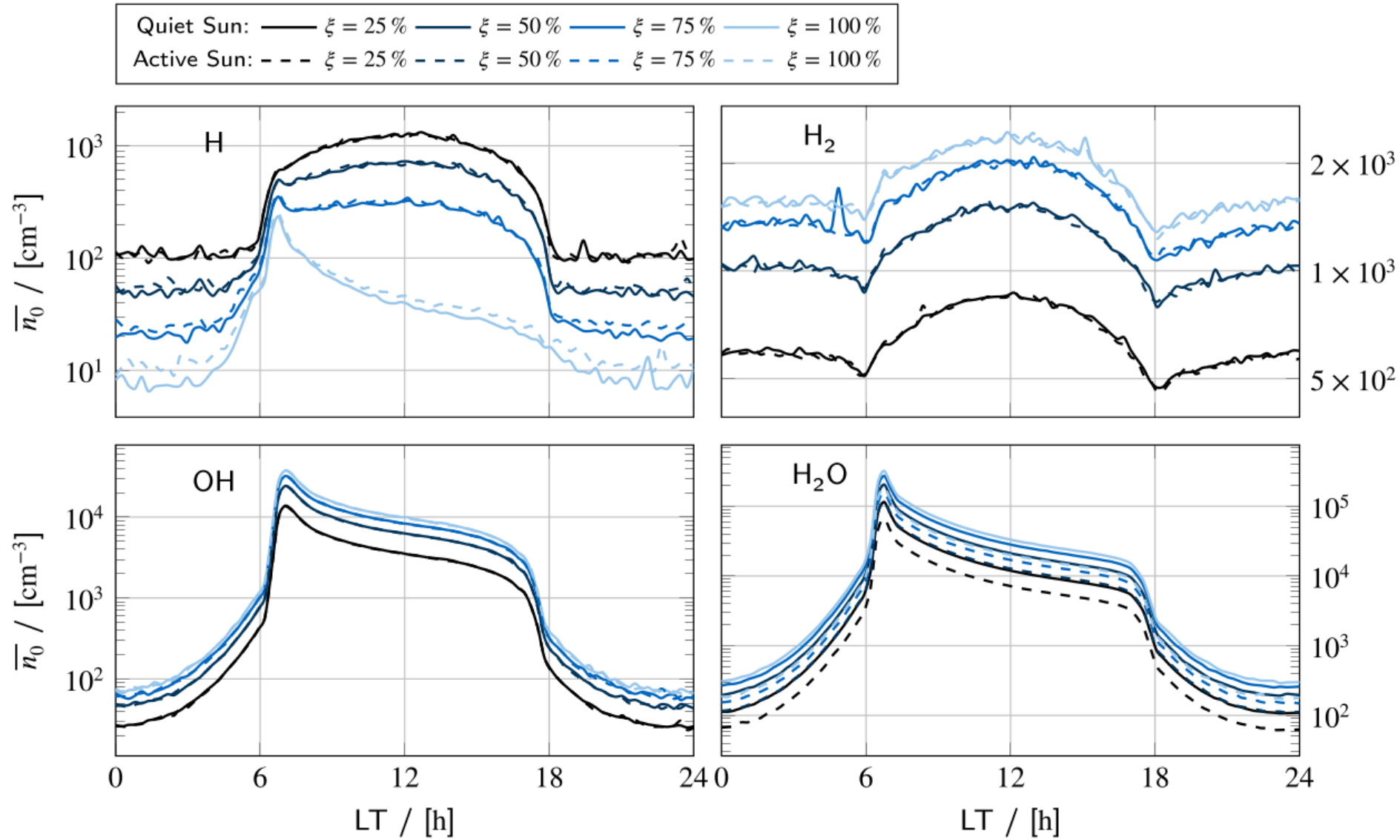
A lot of surface reactivity





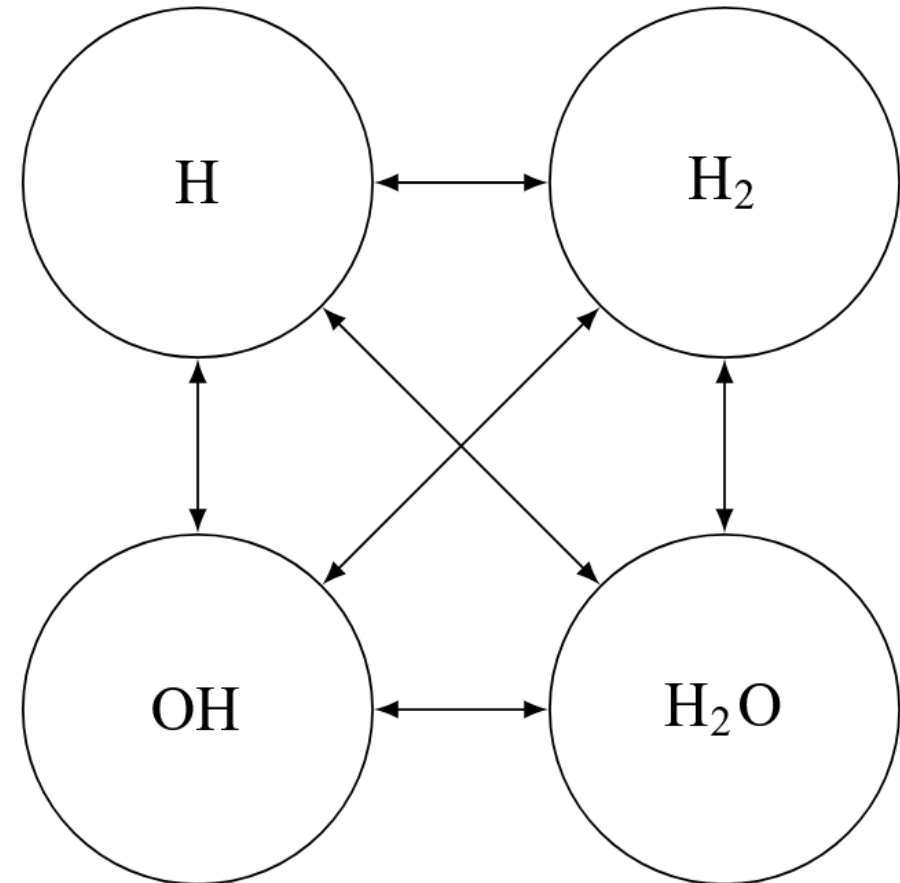
A lot of surface reactivity





Lunar Water Exosphere Simulation

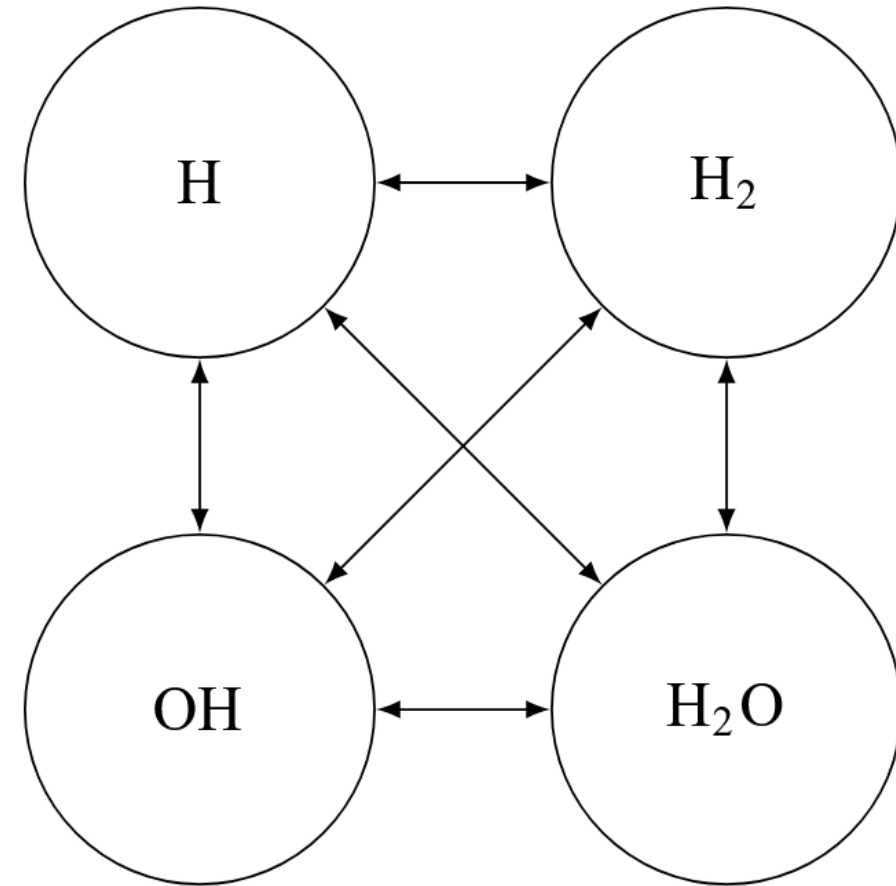
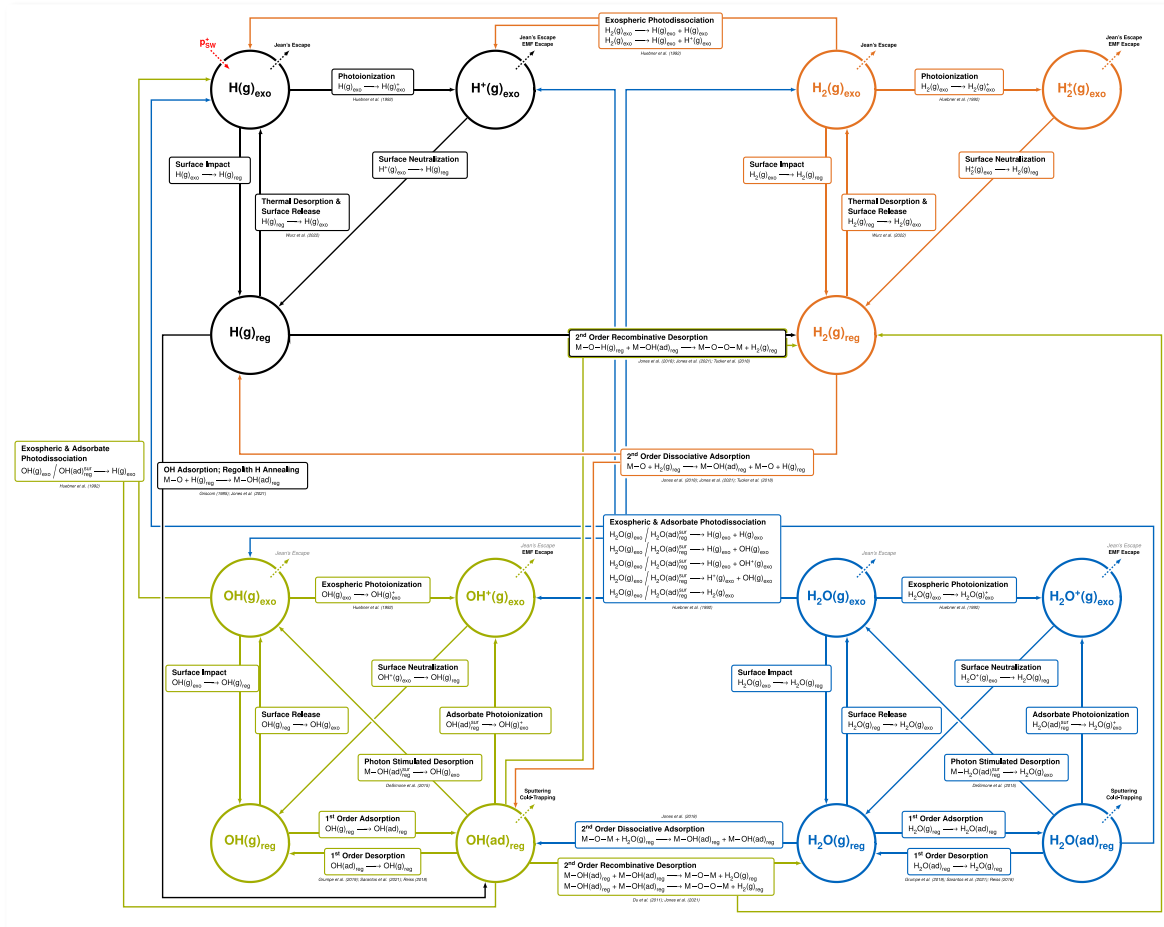
Conversion Reactions



Lunar Water Exosphere Simulation

Conversion Reactions

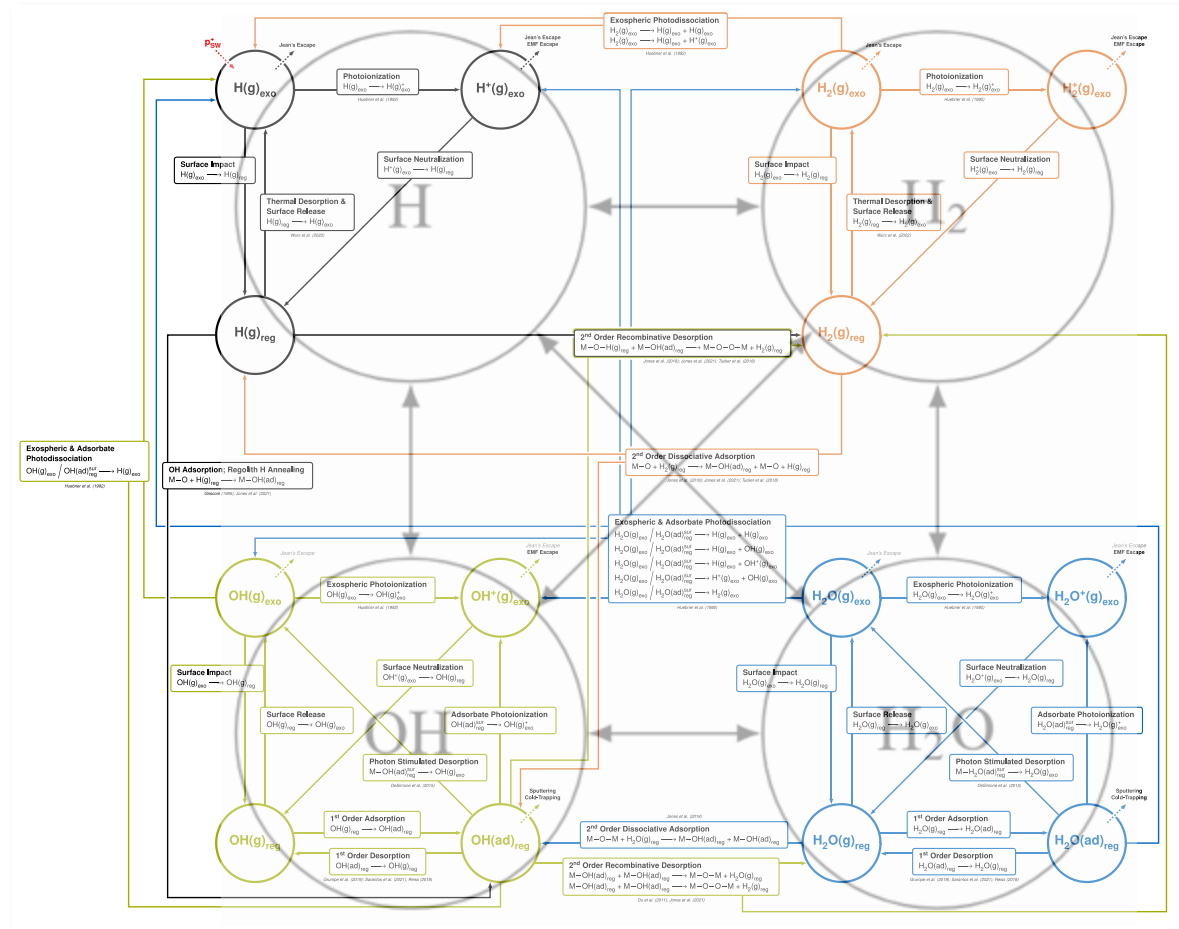
Smolka, 2023 (LPSC)



Lunar Water Exosphere Simulation

Conversion Reactions

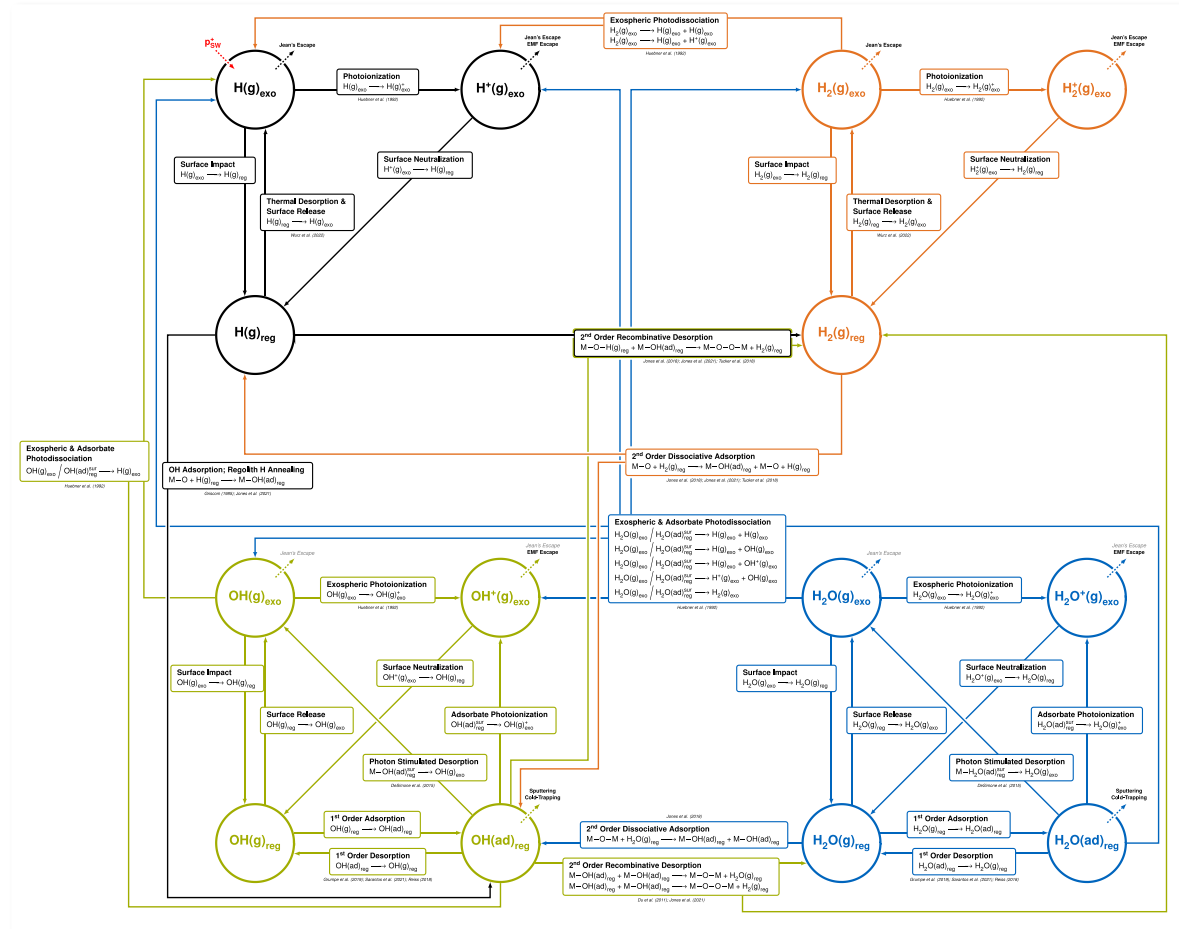
Smolka, 2023 (LPSC)



Lunar Water Exosphere Simulation

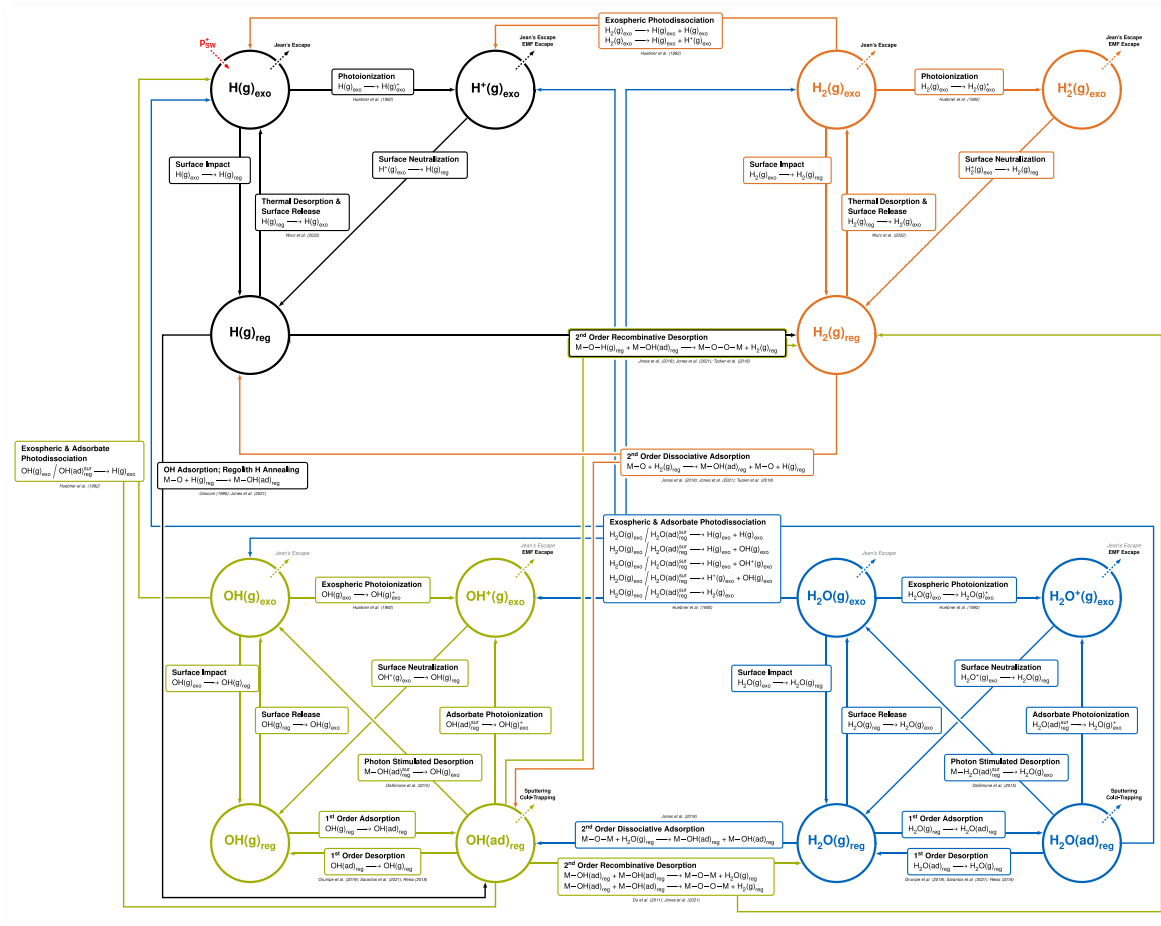
Conversion Reactions

Smolka, 2023 (LPSC)

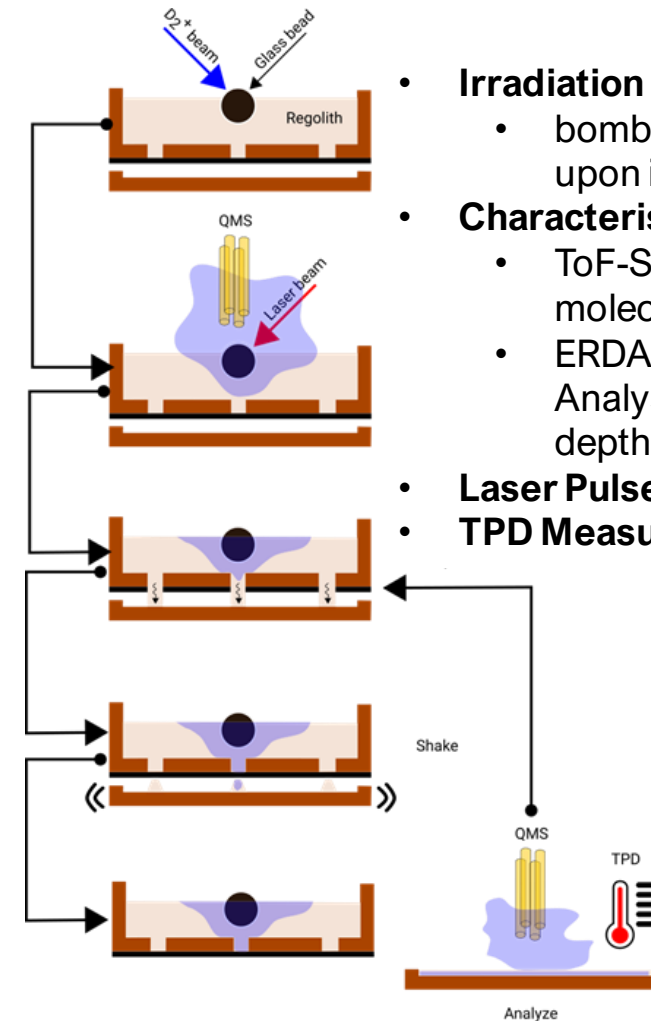


Lunar Water Exosphere Simulation

Conversion Reactions



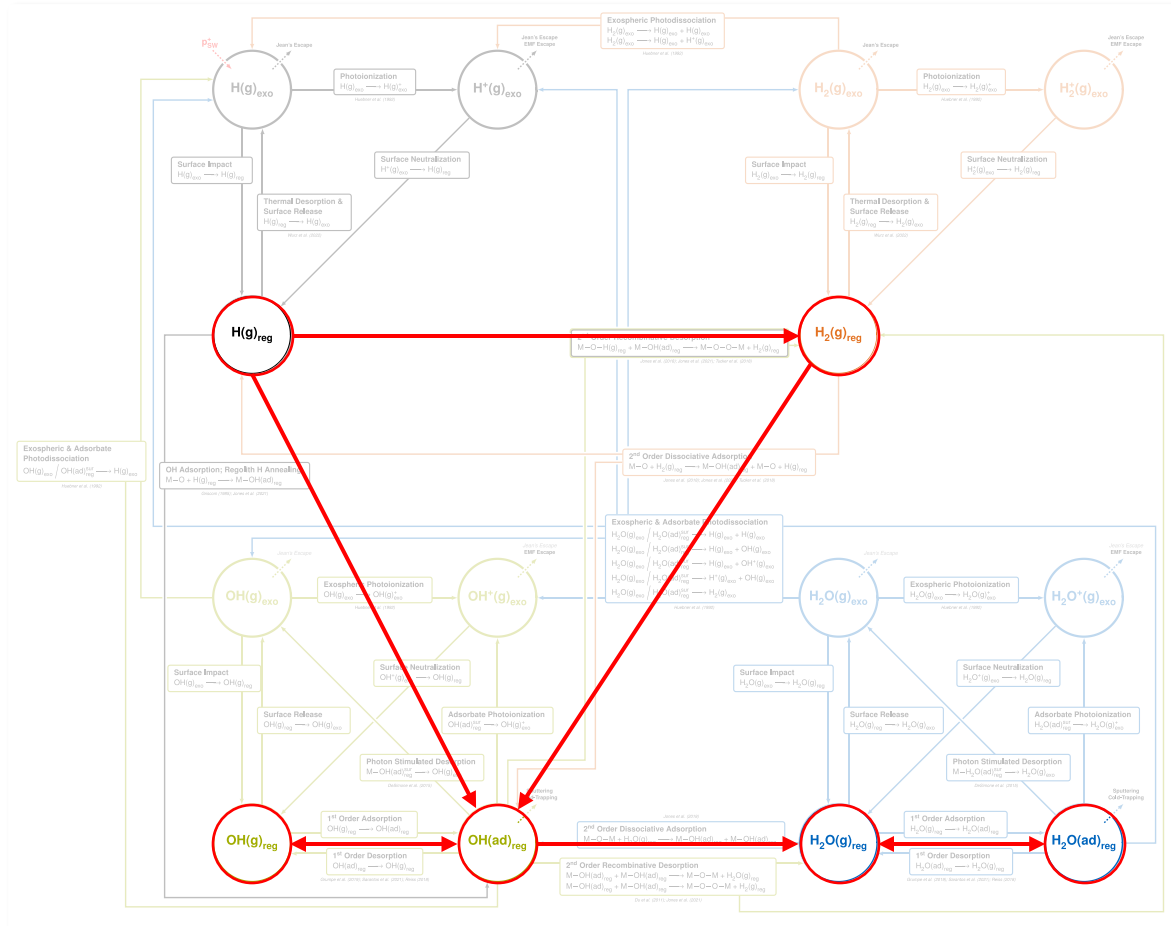
Smolka, 2023 (LPSC)



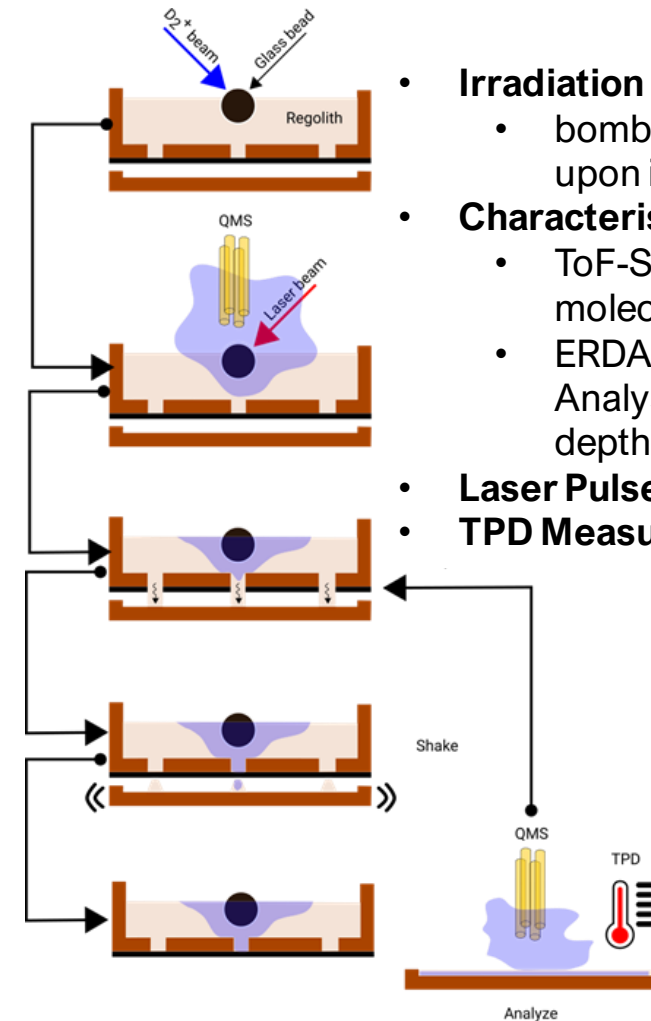
- Irradiation**
 - bombardment with D^+ ; dissociation upon impact
- Characterisation of Irradiated Samples**
 - ToF-SIMS to measure water group molecule concentration
 - ERDA (Elastic Recoil Detection Analysis) to determine deuterium depth
- Laser Pulses to Simulate MMI**
- TPD Measurements**

Lunar Water Exosphere Simulation

Conversion Reactions



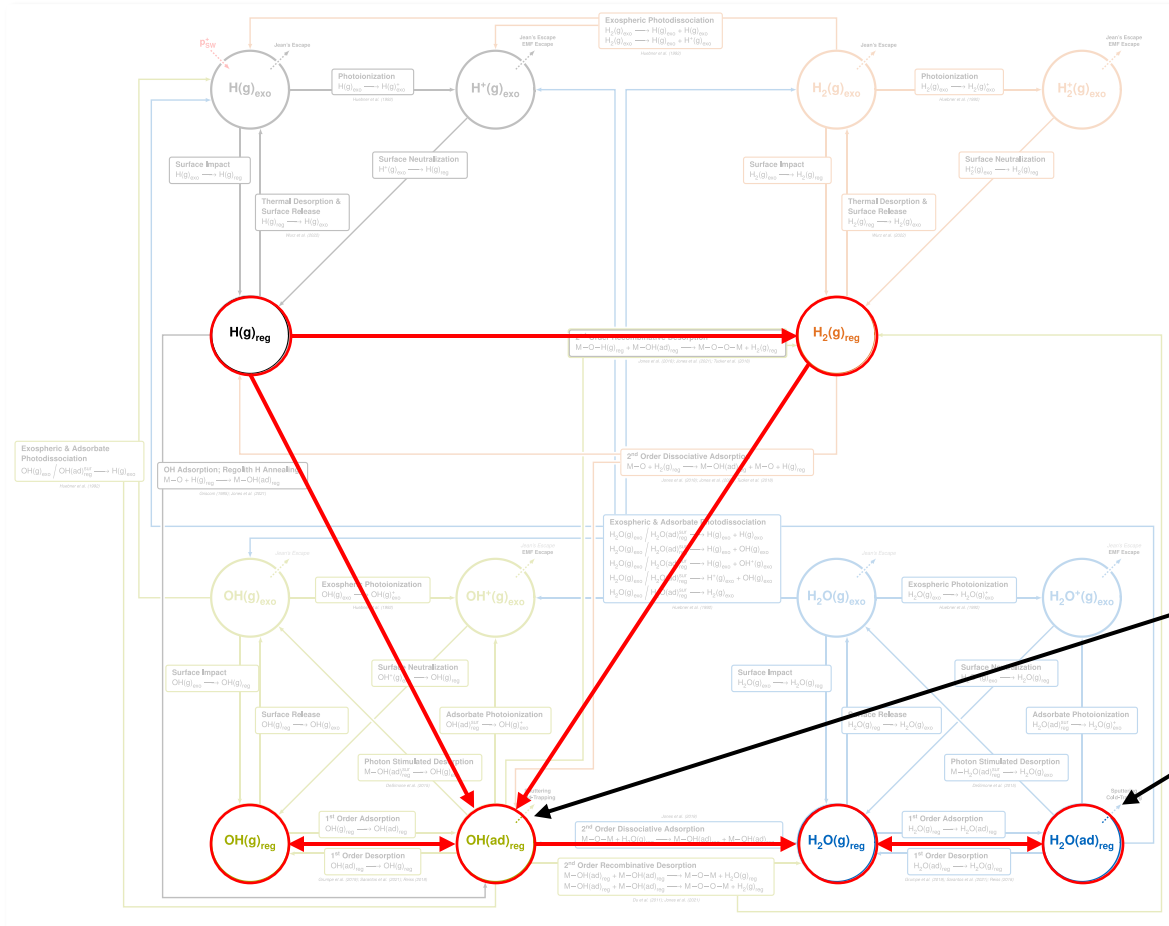
Smolka, 2023 (LPSC)



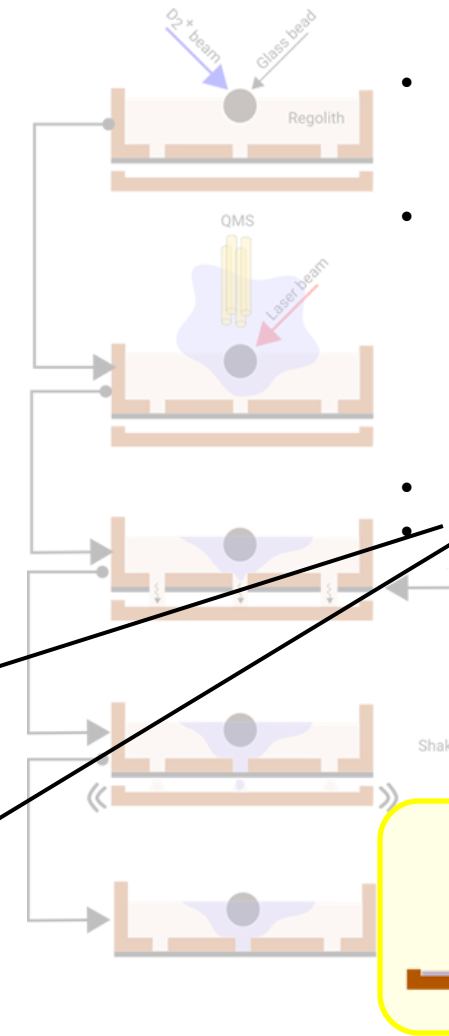
- **Irradiation**
 - bombardment with D+; dissociation upon impact
- **Characterisation of Irradiated Samples**
 - ToF-SIMS to measure water group molecule concentration
 - ERDA (Elastic Recoil Detection Analysis) to determine deuterium depth
- **Laser Pulses to Simulate MMI**
- **TPD Measurements**

Lunar Water Exosphere Simulation

Conversion Reactions



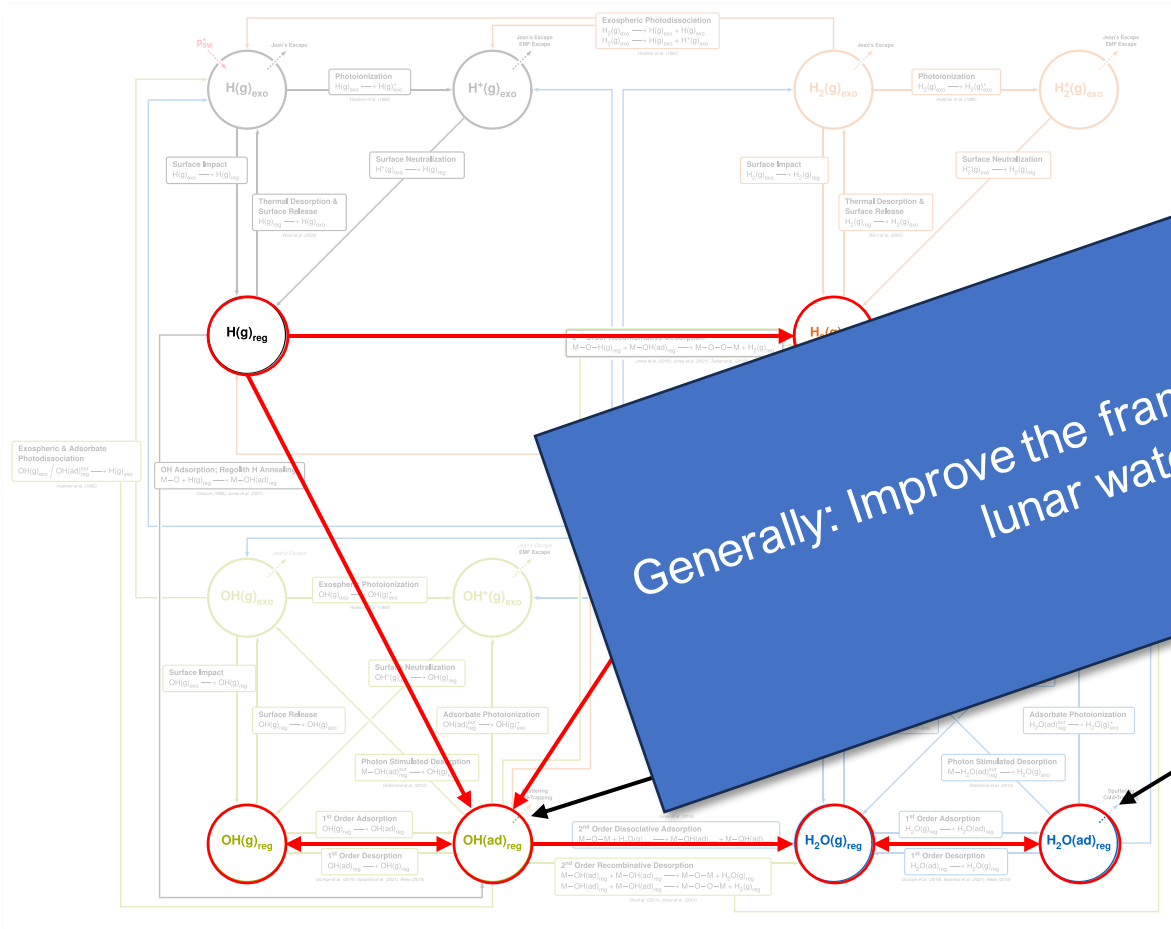
Smolka, 2023 (LPSC)



- **Irradiation**
 - bombardment with D^+ ; dissociation upon impact
- **Characterisation of Irradiated Samples**
 - ToF-SIMS to measure water group molecule concentration
 - ERDA (Elastic Recoil Detection Analysis) to determine deuterium depth
- **Laser Pulses to Simulate MMI**
- **TPD Measurements**

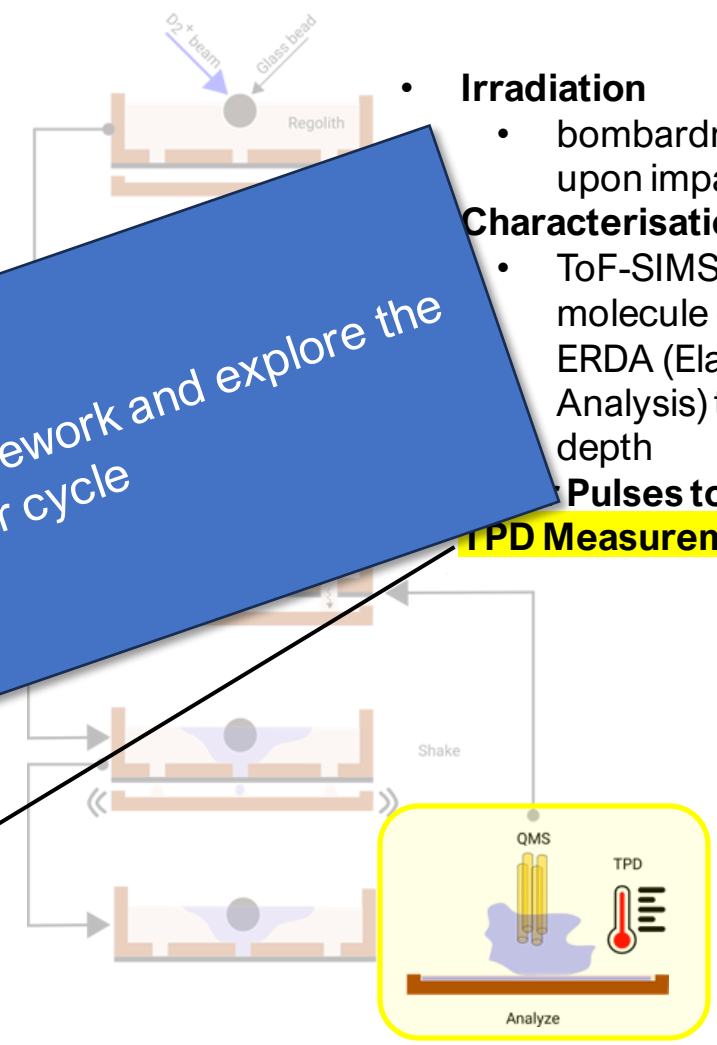
Lunar Water Exosphere Simulation

Conversion Reactions



Generally: Improve the framework and explore the lunar water cycle

- **Irradiation**
 - bombardment with D+; dissociation upon impact
- **Characterisation of Irradiated Samples**
 - ToF-SIMS to measure water group molecule concentration
 - ERDA (Elastic Recoil Detection Analysis) to determine deuterium depth
- **Pulses to Simulate MMI**
- **TPD Measurements**



Smolka, 2023 (LPSC)