Enceladus geyser study using Markov Chain Monte Carlo fits of DSMC simulations

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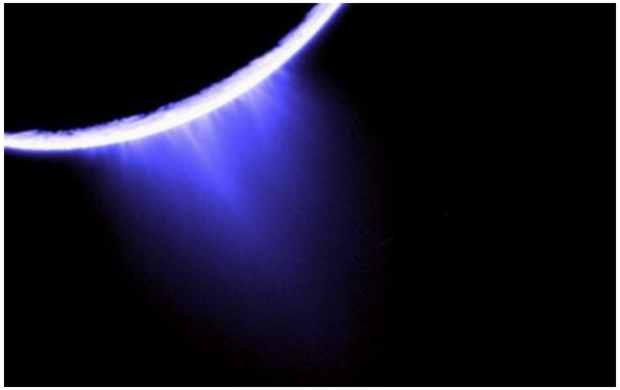
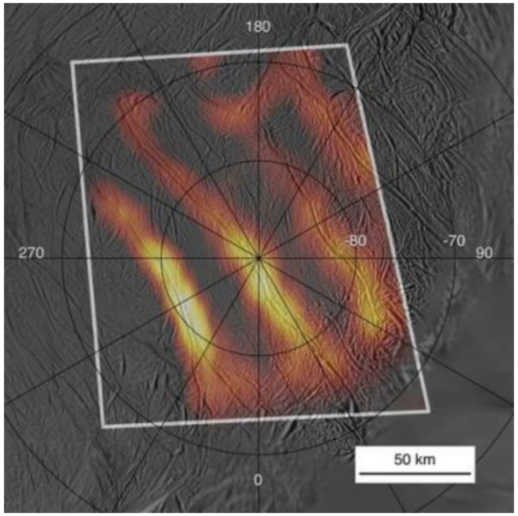
Enceladus and Its South Polar Activity



- 14^{th} moon of Saturn
  - Radius ~250 km
  - Low gravity ~0.113 m/s^2
- One of the brightest objects in the solar system
  - Albedo ≈ 0.99, no atmosphere

- Plume and hot spot detected at South Pole in 2005
- Mixture of water (> 90%), other gases, and icy grains



Credits: Google Maps, NASA/JPL-Caltech, Lunar Planetary Institute, SWRI, SSI

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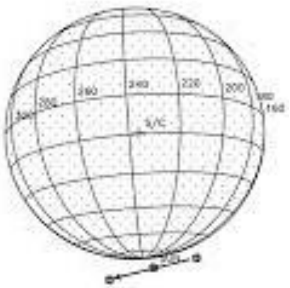
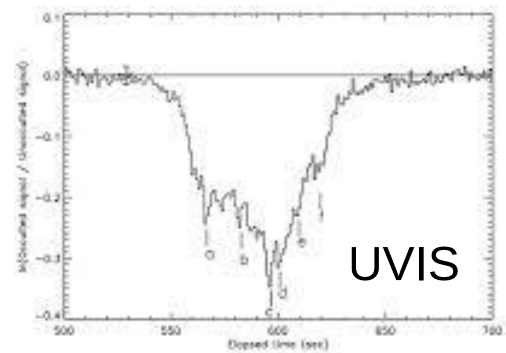
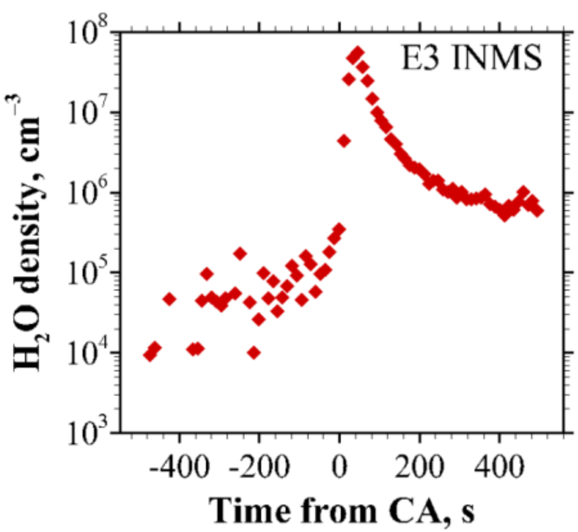
Observations

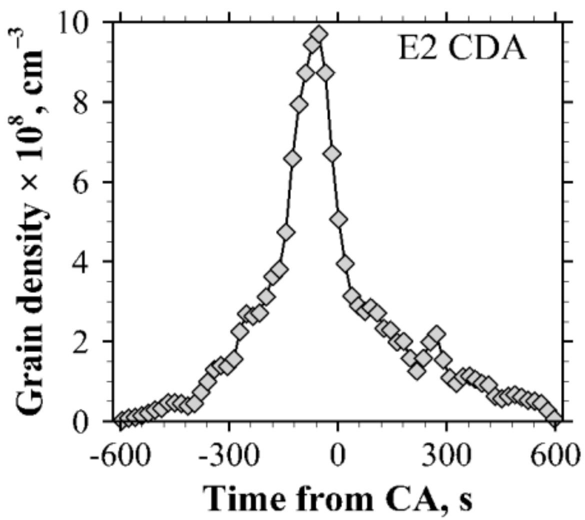
- Different CASSINI instruments observed the plumes
  - **INMS (Mass spectrometer)**
  - **CDA (Cosmic Dust Analyzer)**
  - **UVIS (UV spectrometer)**
  - ISS (Imaging)
  - VIMS (Vis & IR spectrometer)

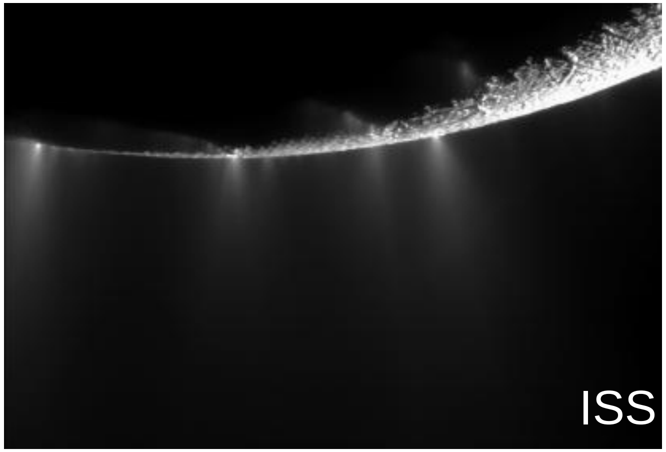
Solar occultation in the UV











Local measurements of H_2O and grains along satellite track

Previous studies

- Authors tried to explain plumes origin and working mechanisms
  - Near-surface explosion of boiling liquid water (Spitale and Porco, 2006)
  - Clathrate decomposition (Kieffer et al., 2006)
  - Evaporation from a underground salty ocean (Porco et al., 2014; Postberg et al., 2009; Schmidt et al., 2008b)
  - How fluids move up the conduits (Kite and Rubin, 2016)
- From observations, studies have tried to constrain the outgassing flow rate and flow characteristics
  - Temperature and speed (Burger et al., 2007; Dong et al., 2011; Hansen et al., 2006; Hansen et al., 2008; Hansen et al., 2011; Saur et al., 2008; Smith et al., 2010; Tenishev et al., 2010; Tenishev et al., 2014; Tian et al., 2007; Waite et al., 2006; Yeoh et al., 2015; Yeoh et al., 2017)
- Plumes studied using different approaches
  - Models using ballistic geysers but ignore outflowing gas is not collisionless in the very-near-field close to the vent (Dong et al., 2011)
  - Assuming analytic solutions to the plume density fields (Teolis et al., 2017)
  - Simple Direct Simulation Monte Carlo (DSMC) approaches (Hedman et al., 2018; Portyankina et al.,2016)

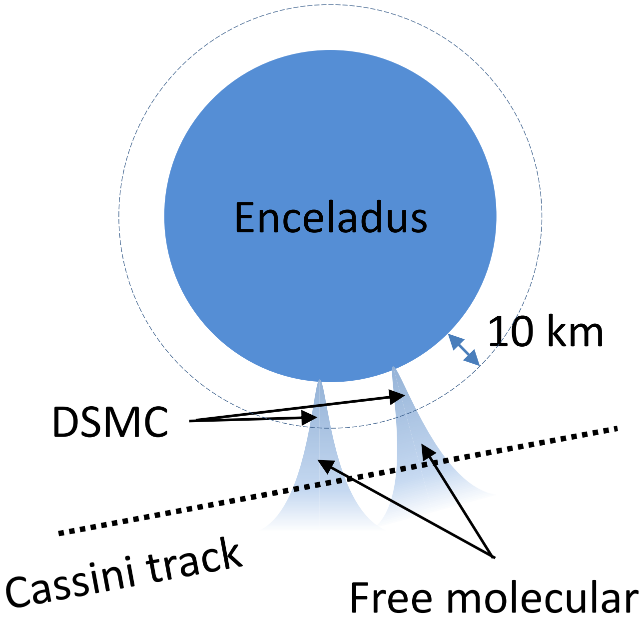
Objectives of the project

- To develop a robust, fast and physically accurate model of the Enceladus two-phase plume via numerical simulation
  - Other models do not treat the important physical processes of plume properly, e.g. change in flow regime, non-equilibrium effects, and interaction between gas and grains, effects of the vent conditions (Yeoh et al., 2015; 2017; Mahieux et al., 2019)

- DSMC modelling from surface to 10 km
- Non-collisional at higher altitude

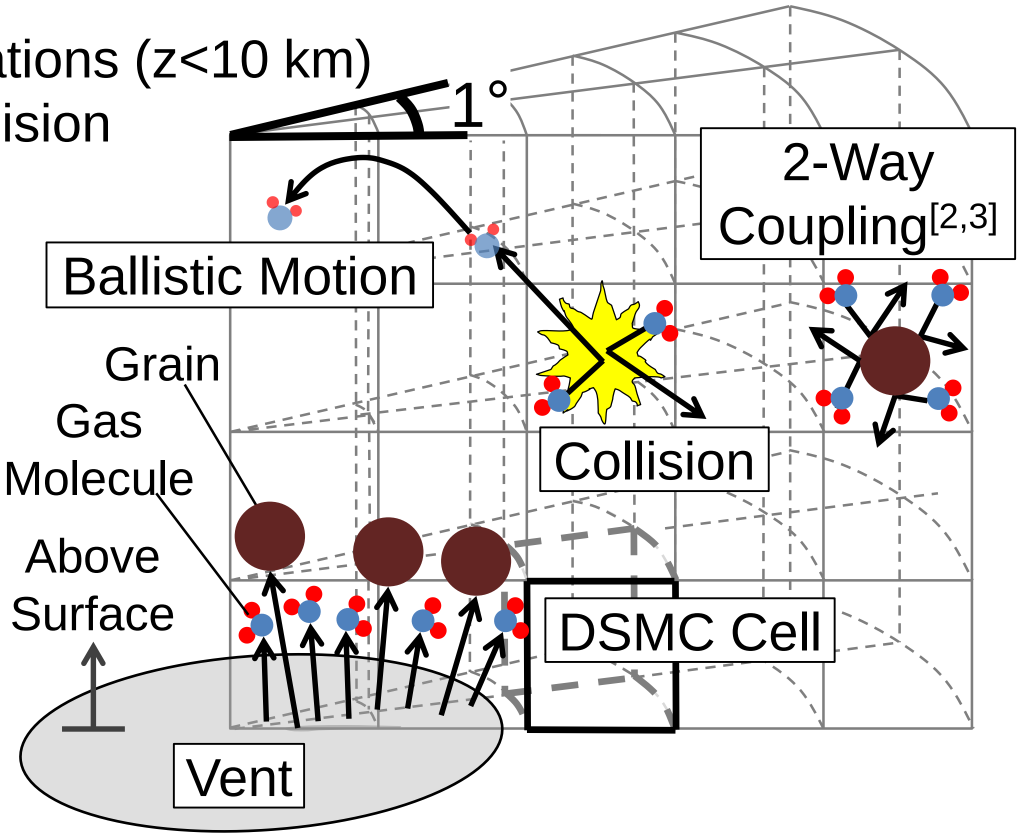
- To study the sensitivity of the vent conditions to the INMS, CDA and UVIS observations (Mahieux et al., *under review*)

- To constrain vent conditions using MCMC (Mahieux et al., *in prep.*)



DSMC close-field calculation approach

- DSMC near field forward simulations (z<10 km)
  - Resolving the molecular collision time & mean free path
- Flow characteristics
  - H_2O gas + water ice mixture expending in vacuum
  - Supersonic flow
- Forces: Enceladus gravity



Default case: Values taken from Yeoh et al., 2015:

Vent radius	Mass flow rate	Gas speed	Ice speed	Ice grain diam.	H_2O/ice ratio	Temp.	Vent exit angle
1.4 m	$13.4 \cdot 10^{-3}$ kg/s	902 m/s	902 m/s	1 µm	95%/5%	53 K	0°

Yeoh et al., Icarus, 2015; 2017

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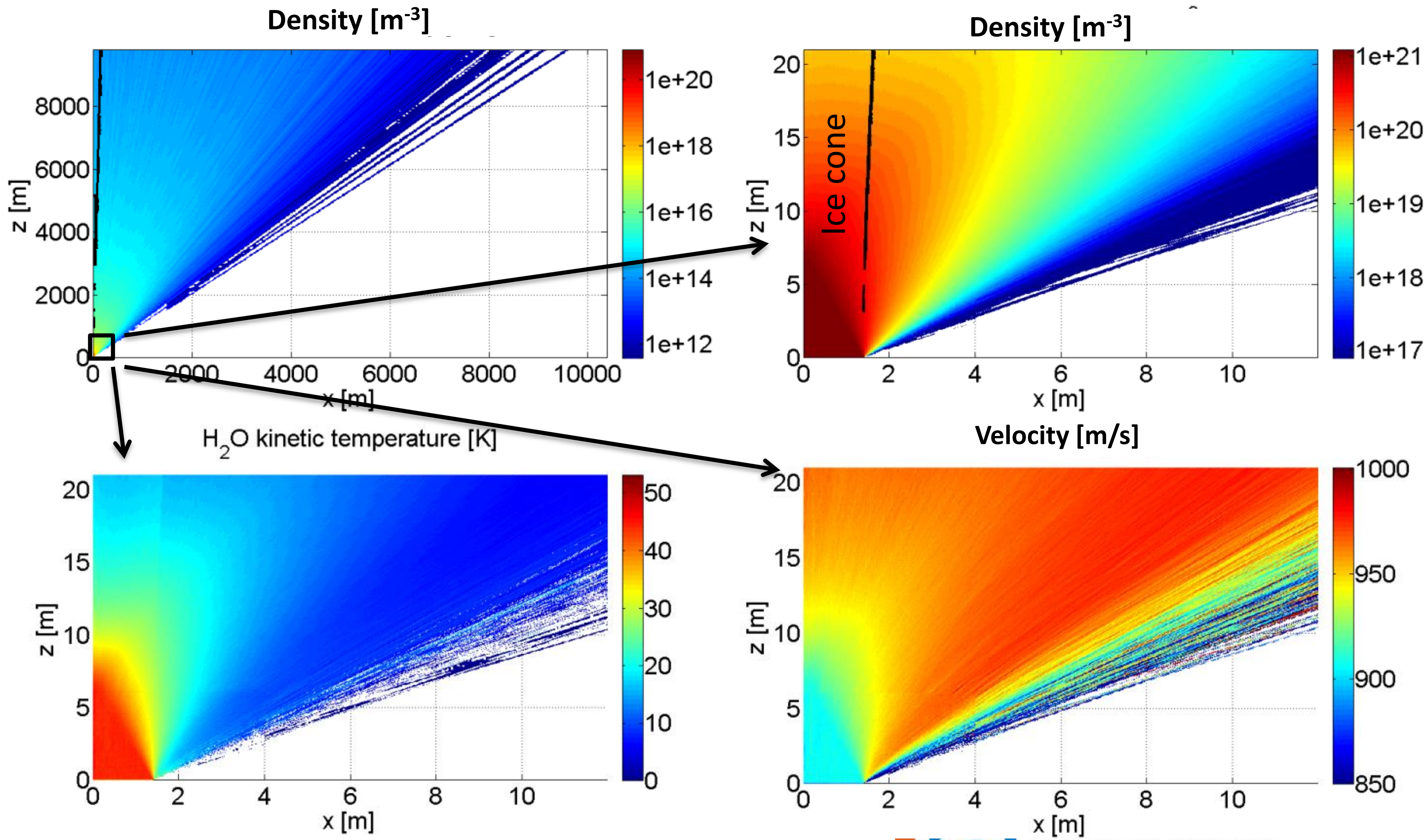
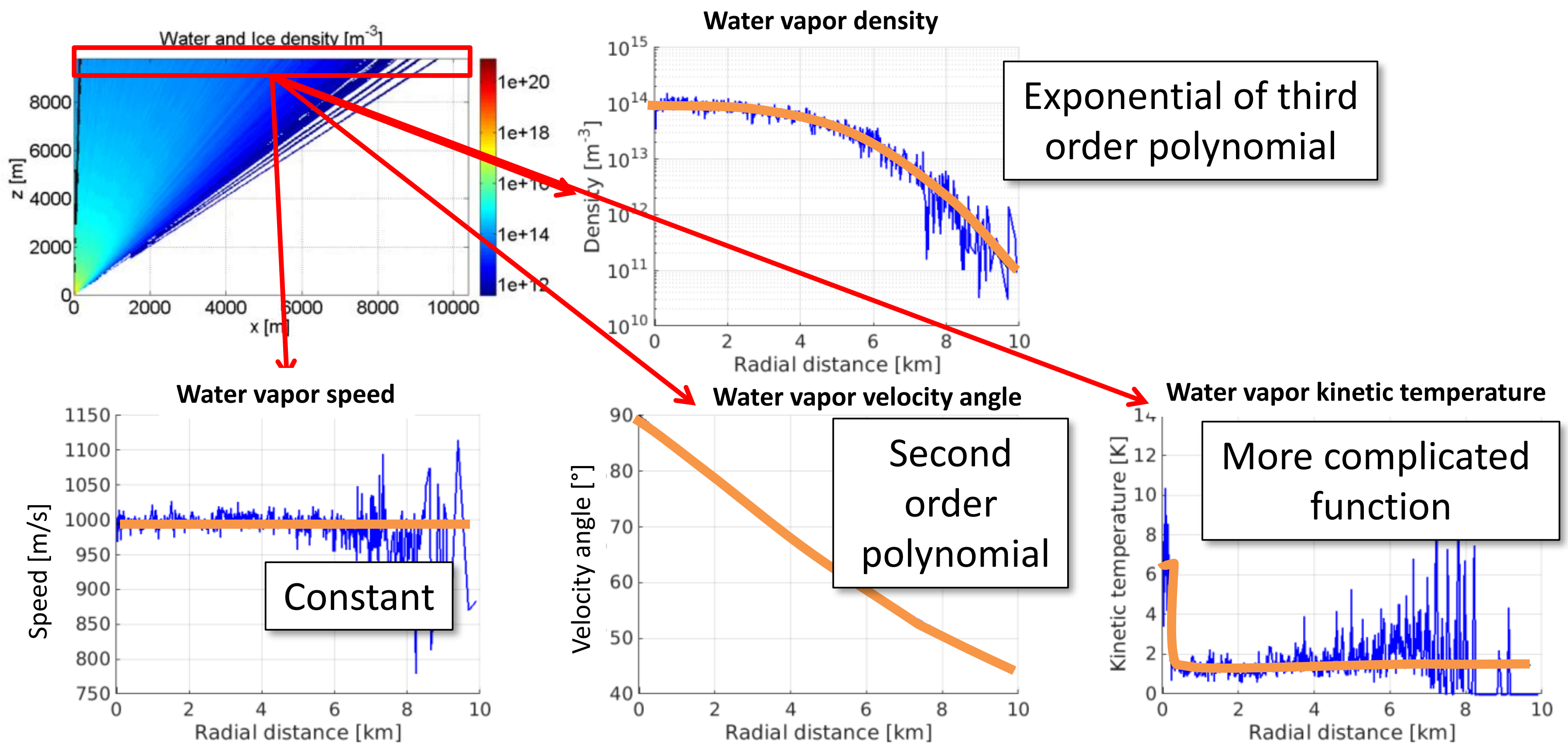
DSMC fields – Default case



Parametric model – Water vapor



- Parameters to study at 10 km:
  - H_2O and ice number density
  - H_2O and ice velocity components (norm and angle to the normal)
  - H_2O and ice kinetic temperature components
  - H_2O rotational temperature

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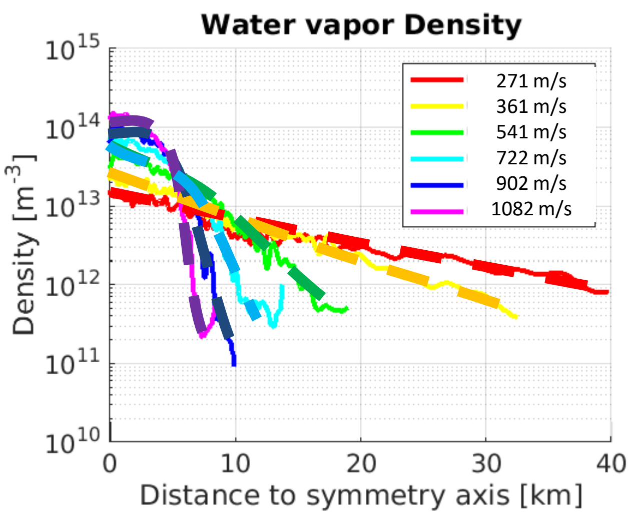
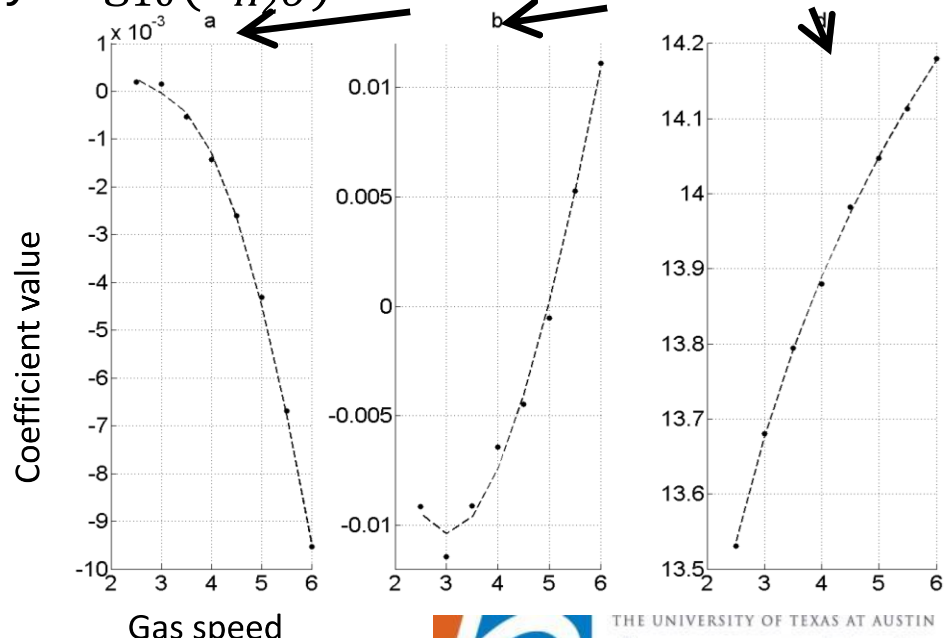
Vent parameters variations

Variations of the parameters: Values taken from literature

	Vent radius [m]	Mass flow [kg/s]	H_2O speed [m/s]	Ice speed [m/s]	H_2O/ice ratio [%]	Flow exit angle	Ice grain size [µm]	Temp. [K]
Min	0.2 m	$13.4 \cdot 10^{-4}$	271	271	100/0	0°	0.01	33
Max	6 m	$13.4 \cdot 10^{-2}$	1082	1082	20/80	9°	5	143
#	21	9	6	6	10	10	5	12

- Example for the H_2O density: $\log_{10}\left(n_{H_2O}\right) = a \cdot x^3 + b \cdot x^2 + d$





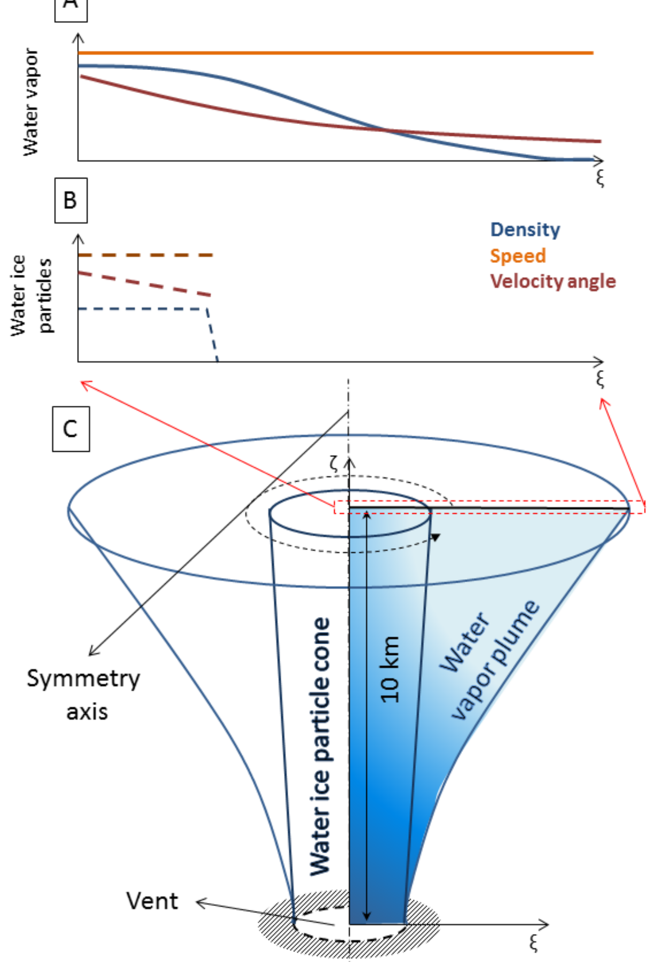
(In)dependence of the vent parameters

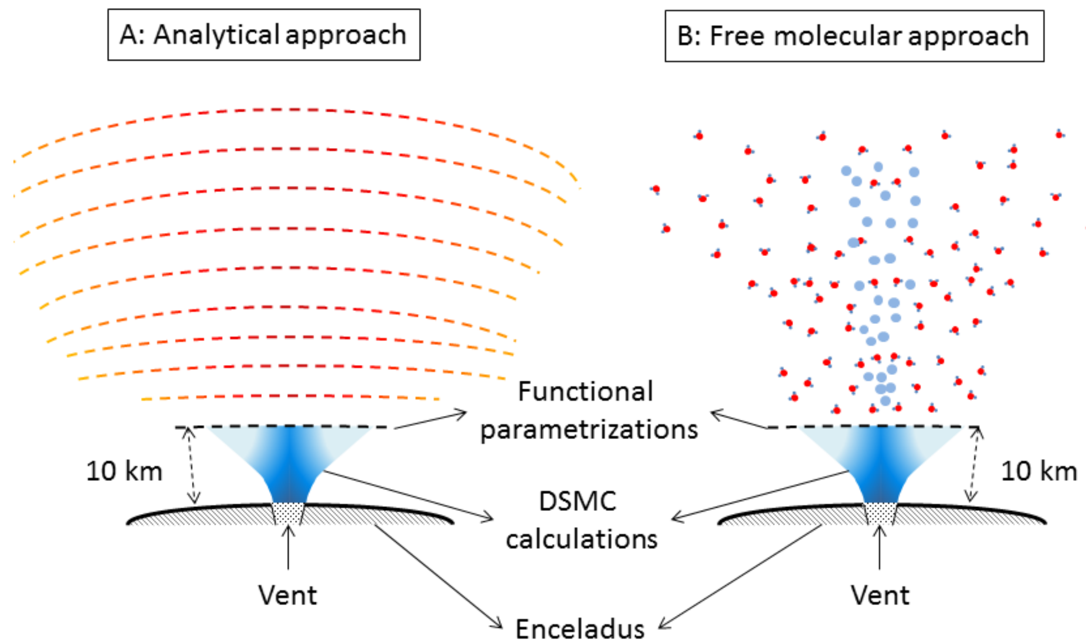
- This approach assumes that the vent parameters have independent effects on the profiles at 10 km
- We can reconstruct the profiles by adding the effects of each variable independently
- This is not true for the speed of water vapor and ice grains
- We consider 2D fits regarding these variables

Propagation of the plumes at higher altitude

- The plumes extend for z >> 10 km
- At z = 10 km, Knudsen number >> 1
  → no molecular collisions

Method used by
Yeoh et al., 2017
(Computationally expensive, not used here)





Analytical expansion of the plume

- Node successive positions obtained by integrating motion equation
- Number density obtained by calculating discrete volumes evolution
- Forces: $\ddot{\boldsymbol{r}} = \boldsymbol{g}_E + \boldsymbol{g}_S + \boldsymbol{a}_E - 2 \cdot (\boldsymbol{\omega}_E \times \dot{\boldsymbol{r}}) - \boldsymbol{\omega}_E \times (\boldsymbol{\omega}_E \times \boldsymbol{r})$

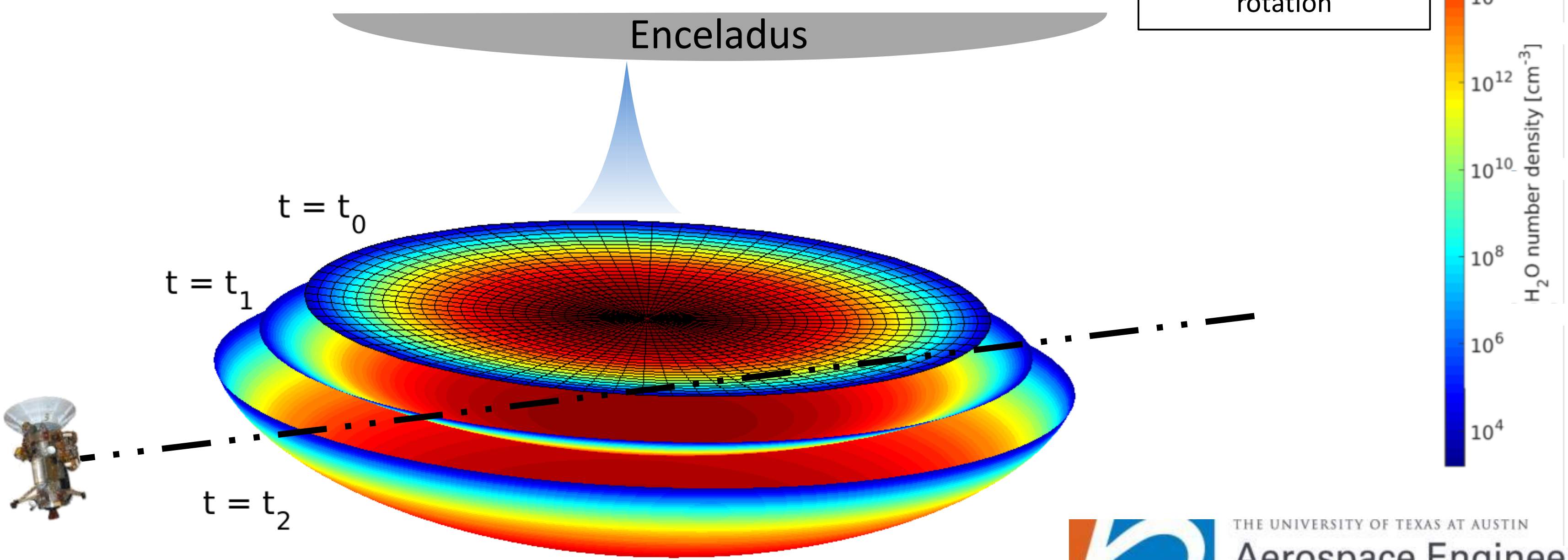
Enceladus gravity

Saturn gravity

Centrifugal acceleration due to the rotation of Enceladus around Saturn

Coriolis acceleration

Centrifugal accelerations due to the Enceladus self-rotation



Fit of all vent parameters of all vents

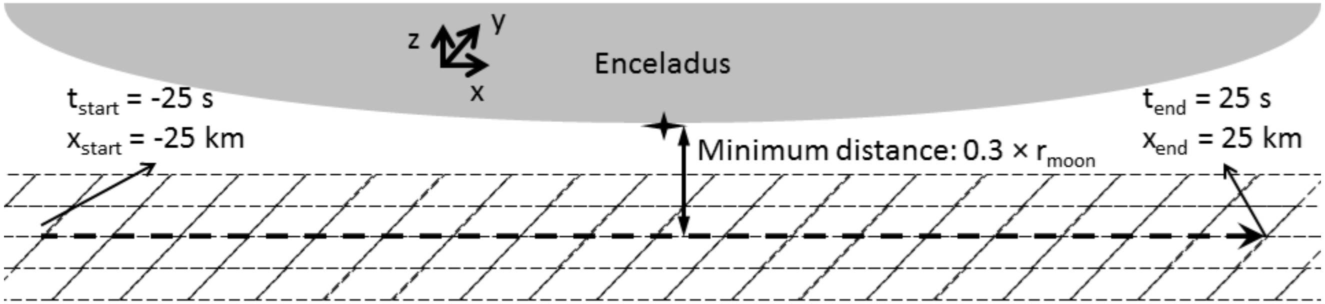
- Vent parameters:

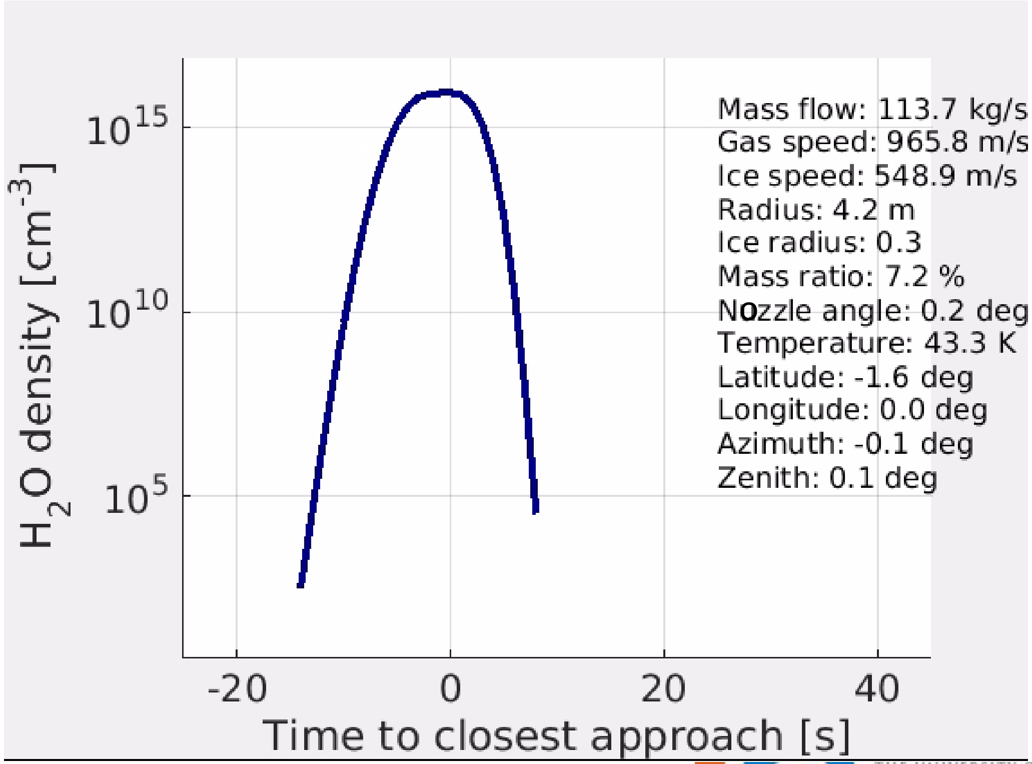
Mass flux	Vent radius	Gas exit speed	Ice exit speed
Mass ratio	Ice particle size	Exit temperature	Exit speed angle
Latitude	Longitude	Zenith angle	Azimuth angle

- For 8 jets (Spitale and Porco, 2006), there are 96 variables
- For 98 jets (Porco et al., 2014), there are **1176** variables
- → The problem is under-constrained
- Some parameters probably play no role
  - E.g. when plume orientation such that the jet never crosses the spacecraft path

  → Monte Carlo sensitivity study to decipher most likely dependent variables
- Build profile database for observation geometry using random values of the vent parameters
- Study correlations between synthetic profiles and vent parameters

Randomly generated profiles





Final size of the sample per vent: 5000

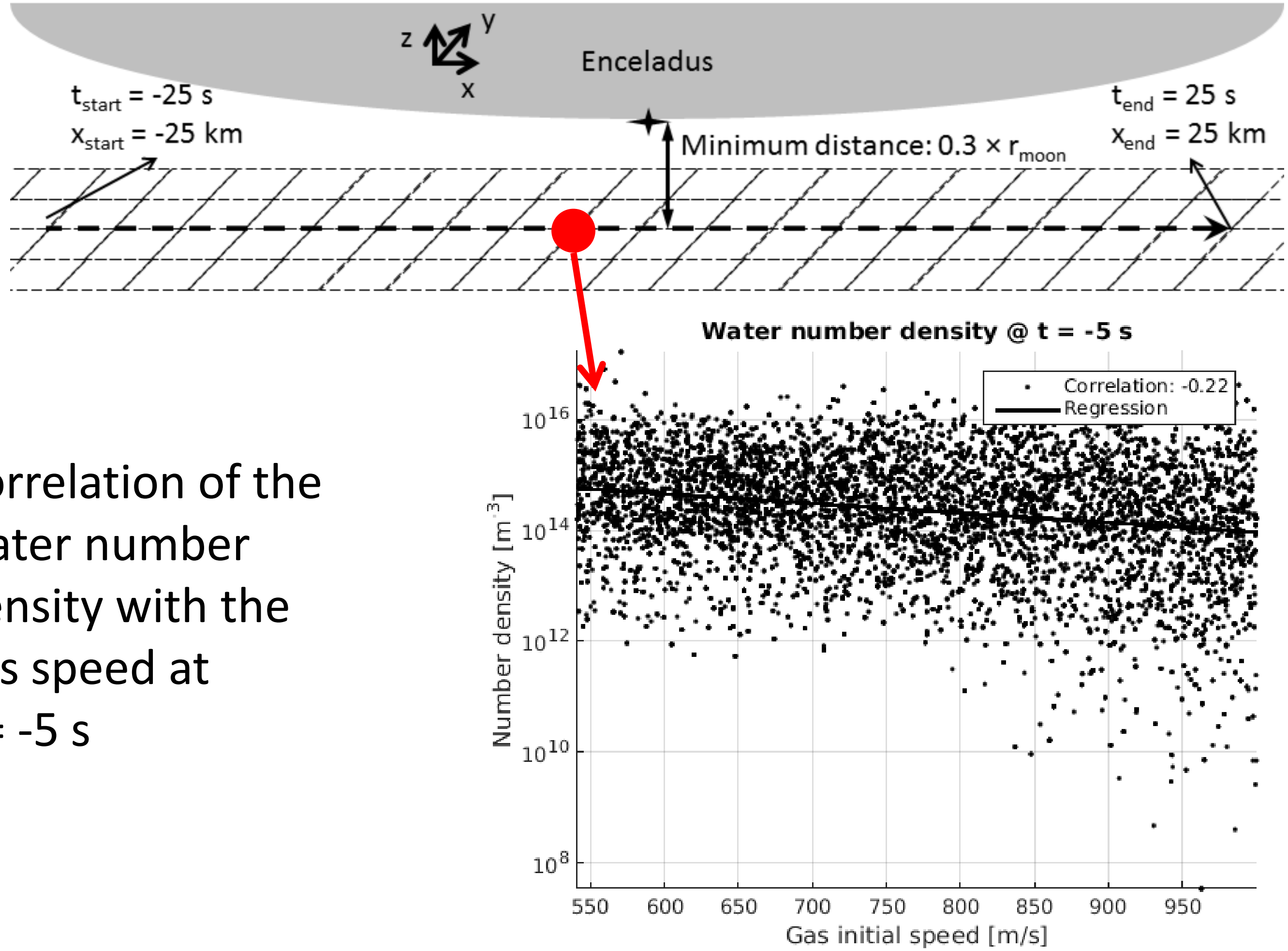
Monte Carlo Sensitivity study: Introduction

- The **Pearson correlation coefficient** ρ_P is a measurement of the linear dependence of one variable upon another variable in a statistical dataset

$$\rho_P = \frac{1}{N-1} \cdot \sum_{i=1}^{N} \left(\frac{X_i - \mu_X}{\sigma_X} \right) \cdot \left(\frac{Y_i - \mu_Y}{\sigma_Y} \right)$$

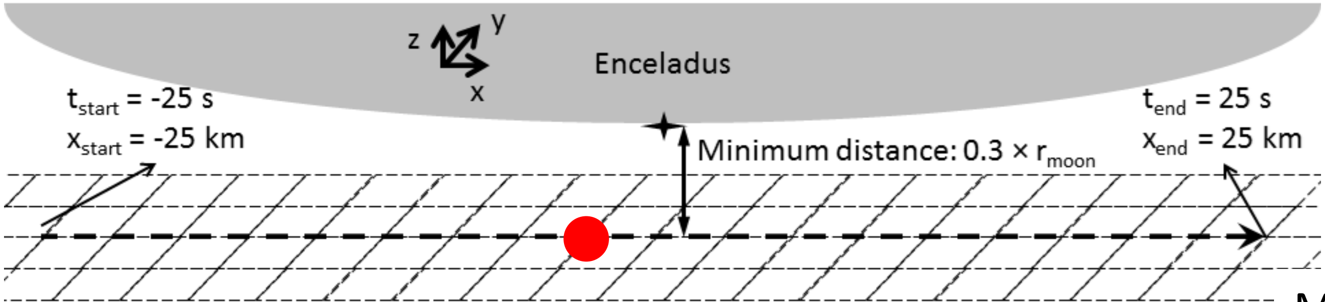
- The Pearson correlation coefficient is associated with the notion of **p-value**, which is a number between 0 and 1 representing the probability that a given data would have arisen if the association between the two variables was random. The p-value is calculated based on a t-distribution.

Calculation of the correlations

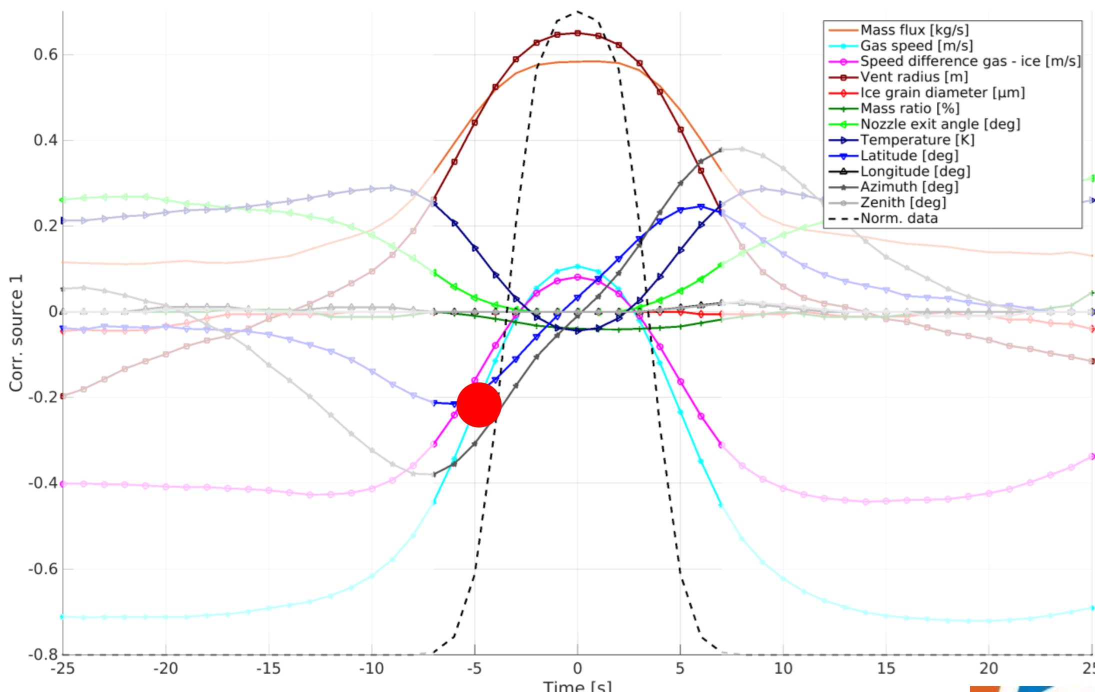


Correlation of the water number density with the gas speed at t = -5 s

Application: Sensitivity to one jet at South Pole



(In bold are the signif. correlated values)



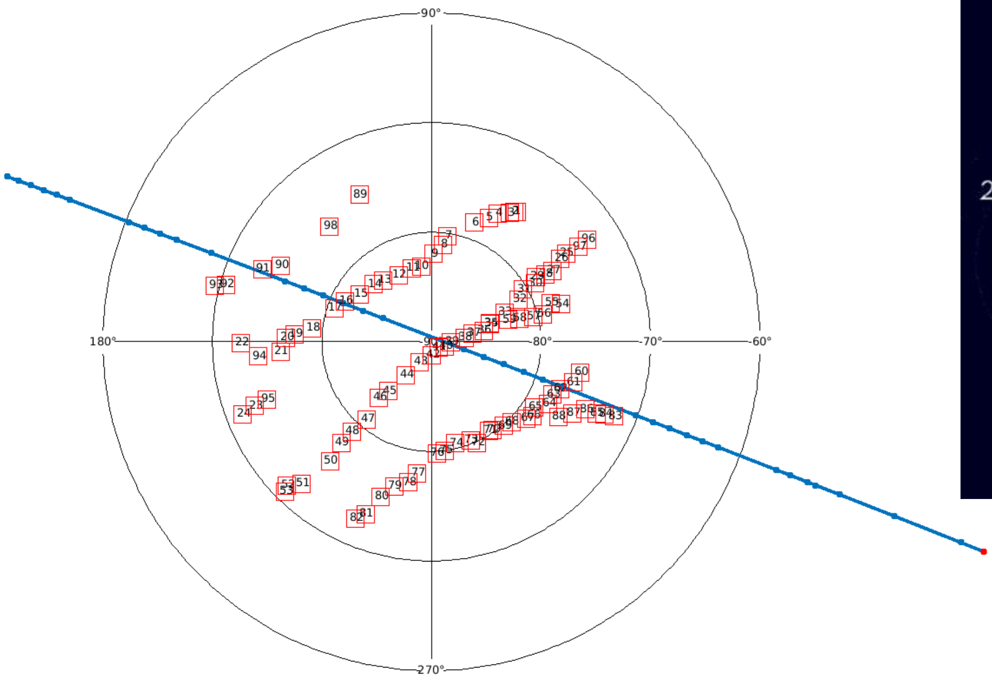
→

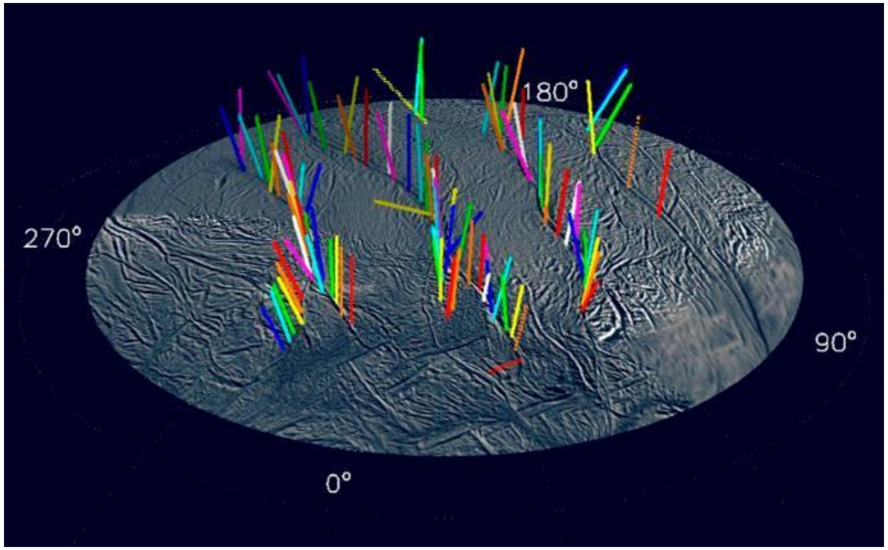
<u>Mean correlations:</u>

Mass flux:	**0.581**
Vent radius:	**0.644**
Gas speed:	**0.108**
Spd diff.:	0.085
Ice grain diam:	0.027
Mass ratio:	0.045
Exit angle:	0.032
Temperature:	0.041
Latitude:	0.085
Longitude:	0.020
Azimuth:	0.096
Zenith:	0.002

Application to INMS observations

- Cassini dataset considered in this work:
  - 7 INMS observations: E2, E3, E5, E7, E14, E17, E18
  - 1 CDA observation: E2
  - 1 UVIS observation: Solar Occultation during E8
- 98-jet location and orientation as reported by Porco et al. (2014)





Spitale and Porco, 2014

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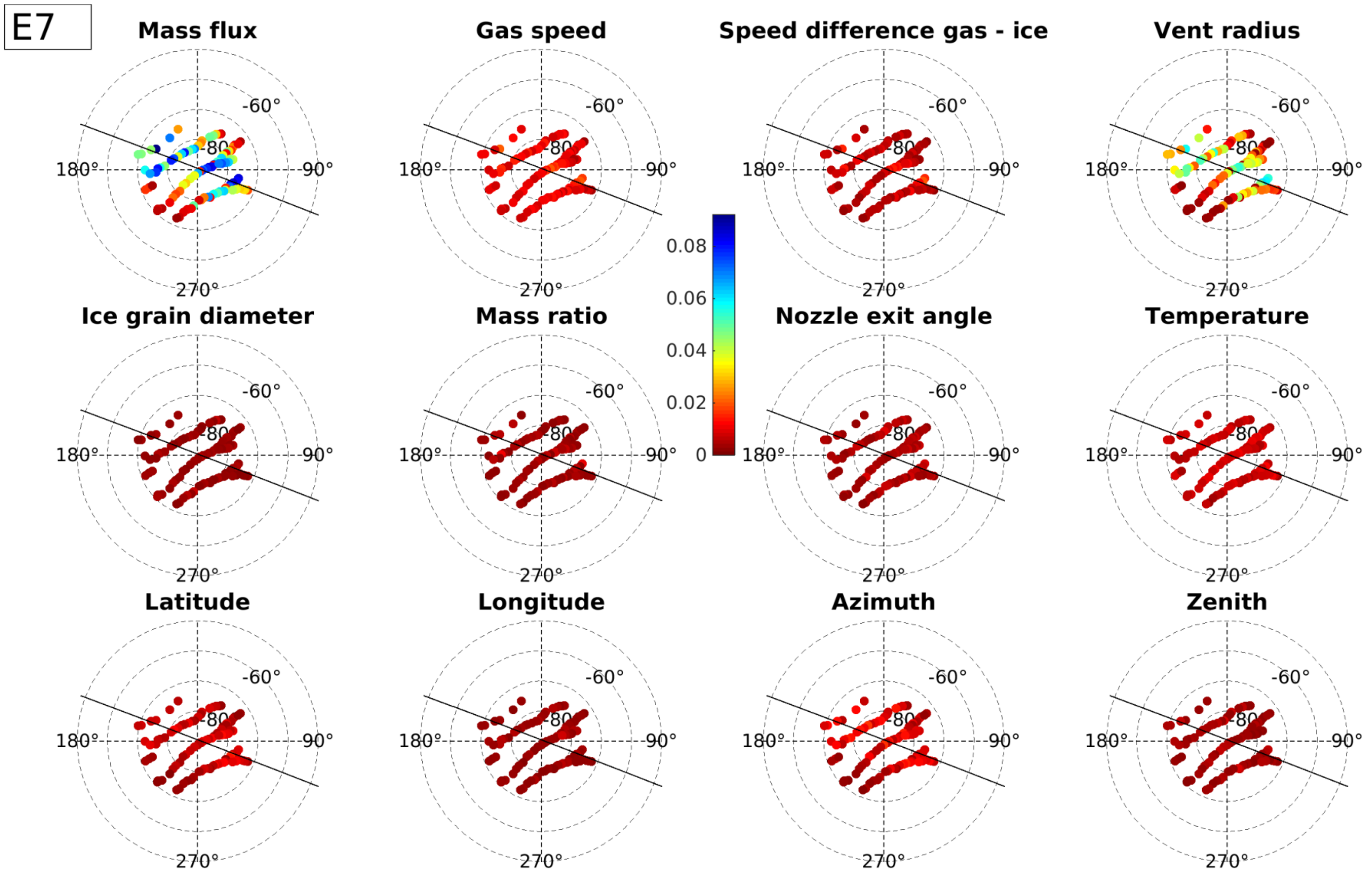
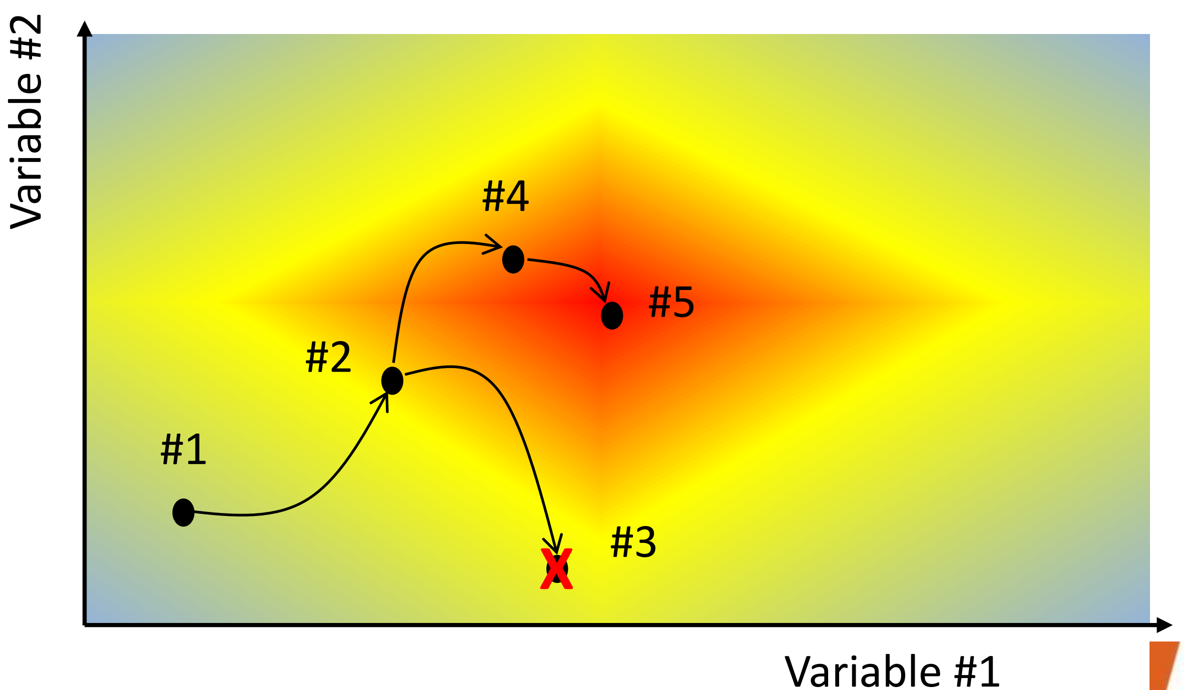
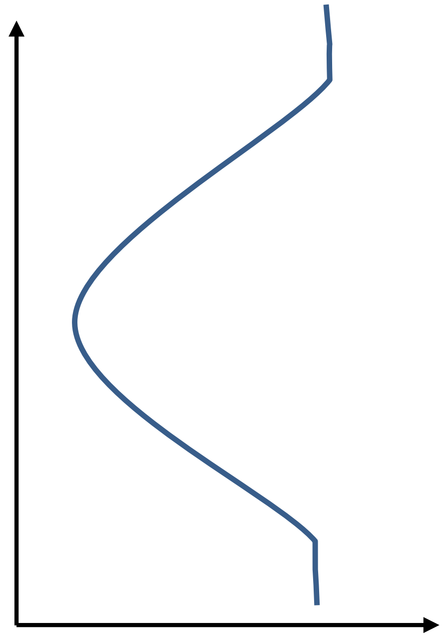
Application to the INMS E7: Mean sensitivity



Markov Chain Monte Carlo principle

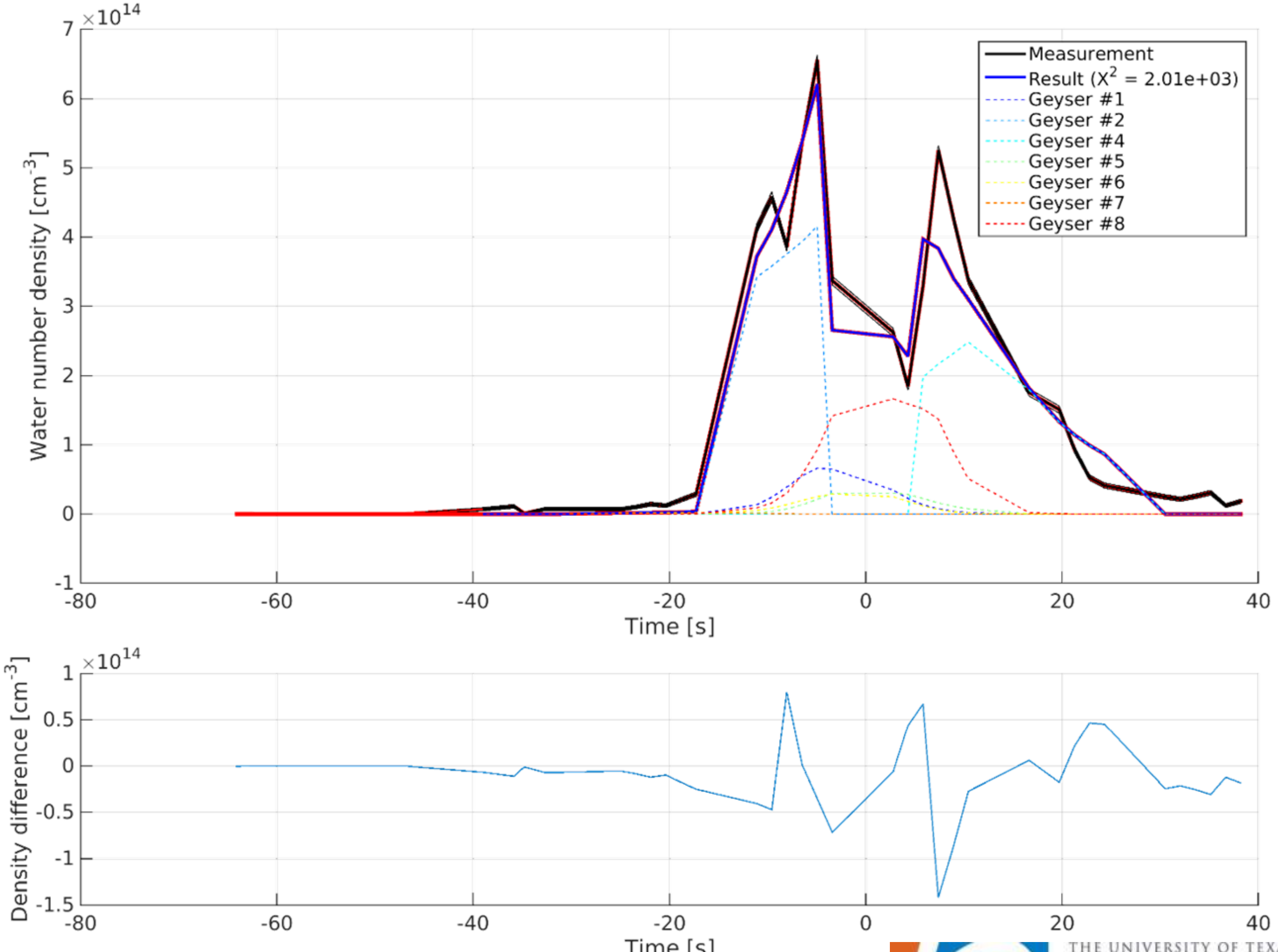
- Algorithm based on random hops in the parameter space and evaluation of a likelihood
- Can handle many variables (>100)
- Needs to calculate many solutions to find the best solution (>10^4)
- Returns likelihood distribution, marginal distributions



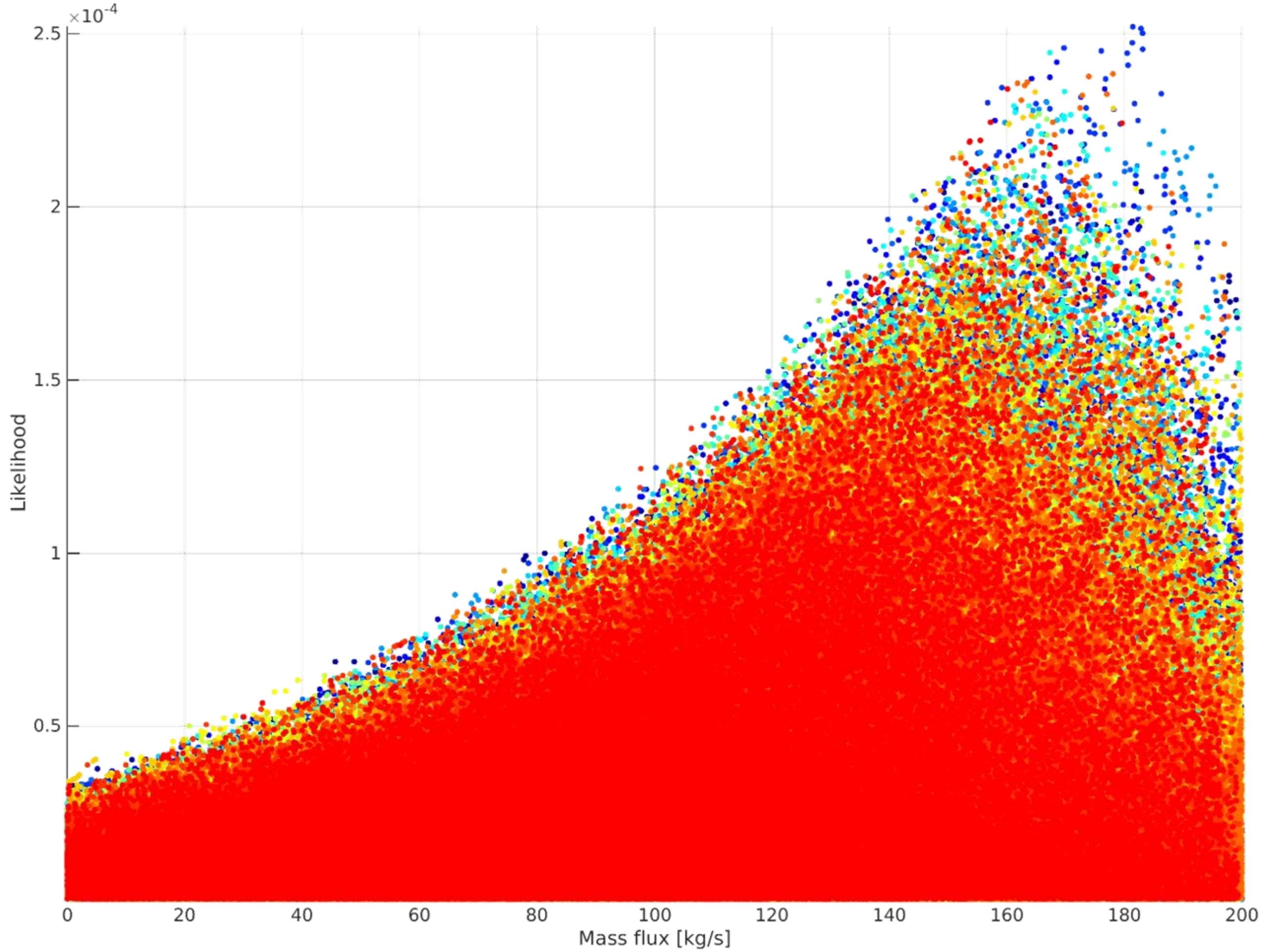


Results for INMS E7, 8 geyser case

- 25 fitted variables



Results for INMS E7, 8 geyser case



Mass flow of sources #2

Conclusions and future prospects

- **Parametrization using functional forms**:
  - New way to generate reliable profiles for free molecular flow without running DSMC
  - Can be applied to other bodies: comets, Europa, engineering rocket applications, …
- Method is **faster by 3 orders of magnitude** (5 days to 1 s)
- Returns **density and velocity fields** without stochastic noise
- Sensitivity method returns the list of parameters the problem is sensitive to and to which extent, <u>but</u> it is only a rejection criterion
- Markov Chain Monte Carlo fits returns likelihood distribution
  - 8 sources with 25 free parameters presented here
  - 98 sources with >100 free parameters being computed