RPC 2020

Virtual Research Presentation Conference

Hypervelocity Sampling Across the Solar System: Retiring Risks for Enceladus/Europa (Task 1)

Principal Investigator: Morgan L. Cable (3225)
Co-Is: Many (see slide 10 for complete list)
Program: Strategic Initiative

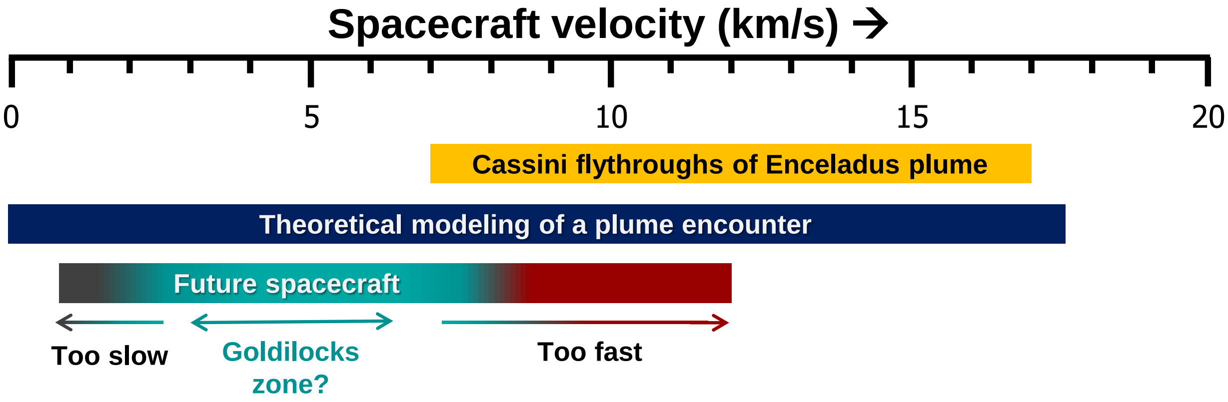
RPC-088

Jet Propulsion Laboratory
California Institute of Technology

Does Plume Sampling Have a Speed Limit?

Abstract

We aim to understand what happens when an ice grain (containing organic molecules) hits a surface at hypervelocity. This is important for a future mission that would search for life at Enceladus by flying through the plume at speeds up to 5 km/s. If biosignatures are trapped within the ice grains of the Enceladus plume, we must prove that we can identify and quantify them after impact.



Spacecraft velocity (km/s) →

Cassini flythroughs of Enceladus plume

Theoretical modeling of a plume encounter

Future spacecraft

Too slow

Goldilocks zone?

Too fast

When an ice grain hits a metal surface at 5 km/s, it vaporizes (goes ‘poof’) and ionizes many of the molecules from the grain in the process. This is called **impact-induced ionization** and is a great way to give molecules a charge, so they can be detected by an instrument like a mass spectrometer (which can only detect ions, not neutral molecules). If the ice grain is moving too slowly, there is not enough energy to ionize the molecules upon impact. If it hits too fast, the molecules may start to fragment into smaller pieces, making it hard to identify what was originally there.

Our goal with this project (completing Year 2 of 3) is to determine the best speed to sample the ice grains of Enceladus such that the biosignature molecules we are looking for (amino acids and fatty acids) are ionized but not fragmented.

Pre-decisional: For Discussion Purposes Only

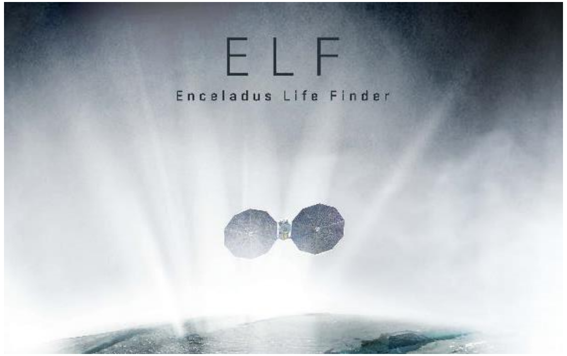
Problem Description

Context

Goal: Address a weakness from our previous Enceladus New Frontiers (NF-4) proposal:

“The proposed investigation assumes that amino acids and fatty acids remain intact after the 5 km/s impact collision required to collect the host ice grains, but there is not much evidence presented that this will be the case in practice.”

We are providing this evidence to support efforts to propose a similar mission to Enceladus in NF-5.



State-of-the-Art (SOA)

Currently, no experimental system exists that can accelerate ice grains (of the correct size and composition) to 5 km/s and analyze the result *in situ*. **We are building two such systems.**

Also, no theoretical simulations have ever attempted to model impacts of large ice grains containing biosignatures onto a surface, as this requires modeling millions of molecules and significant computational resources. **Our team has done this for the first time.**

Relevance

If we want to win a mission to Enceladus in the next New Frontiers round, we must convince reviewers that (1) molecules of interest to astrobiology are preserved after hypervelocity impact, and (2) we can use mass spectral analysis to distinguish between biotic and abiotic compositions. We are on track to have both experimental and theoretical validation of these objectives.

Our work is positioning JPL as the lead U.S. center for testing and developing instruments to sample ice grains at hypervelocity, relevant for Enceladus, Europa, comets, and other Ocean Worlds.

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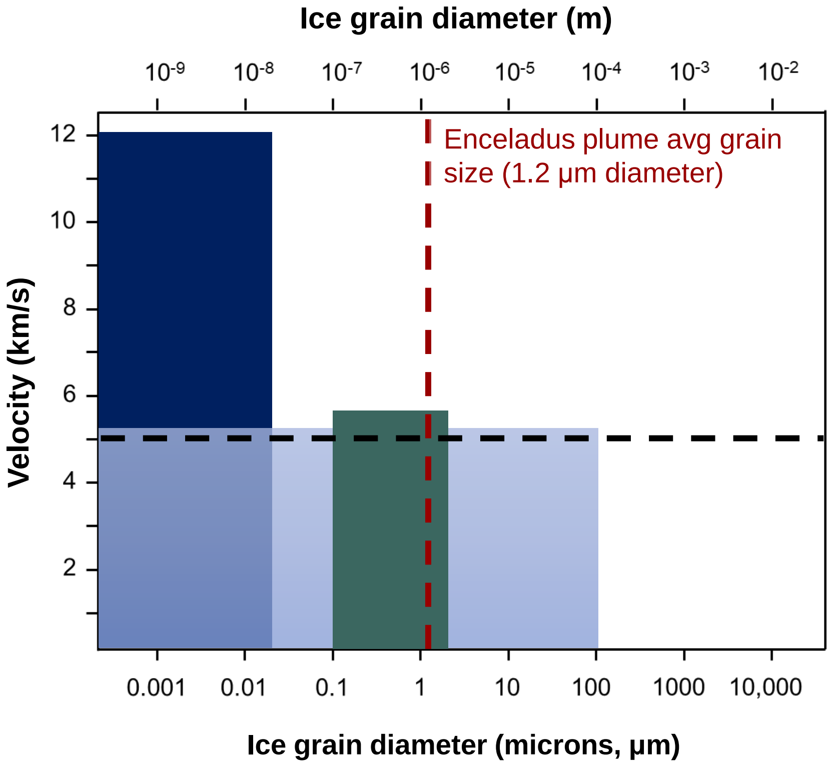
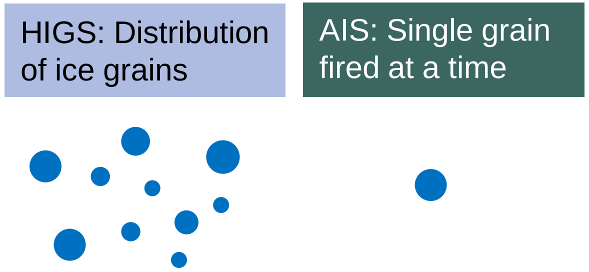
Methodology



- 🟦 Hypervelocity Ice Grain System (HIGS) at JPL
- 🟩 Aerosol Impact Spectrometer (AIS) at UCSD
- ■ Theoretical Modeling at Caltech

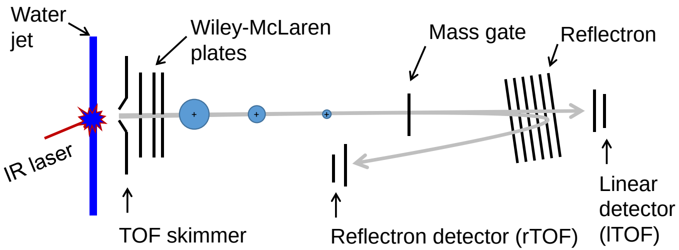
ELF Flyby Speed (proposed, 5 km/s)

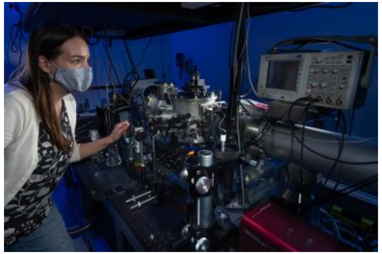


Methodology

Hypervelocity Ice Grain Setup (HIGS)

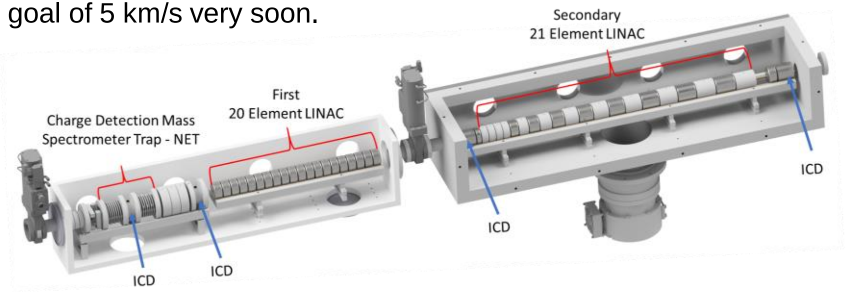
We use an IR laser fired at a water beam to generate a distribution of water clusters and droplets, which freeze to generate ice grains of various sizes. These are traveling at 3-5 km/s and are detected using a time-of-flight (TOF) mass spectrometer. By dissolving salts and biomolecules in the water beam, we can generate ice grains similar to the Enceladus plume.





Aerosol Impact Spectrometer (AIS)

AIS uses electrospray ionization to generate charged ice grains. A single grain is trapped in an electrostatic trap, and its mass and charge are measured. Then it is fired through two linear acceleration stages to reach hypervelocity. We have currently reached 3.7 km/s with this system, and are on track to reach our goal of 5 km/s very soon.



Theoretical Modeling at Caltech

We use high-fidelity reactive molecular dynamics (RMD) simulations to determine at what velocity biomolecules begin to fragment. These simulations are run at different velocities (1-12 km/s), impact angles and orientations. We also generate fragmentation pathways to understand what is happening to the molecules at higher speeds.

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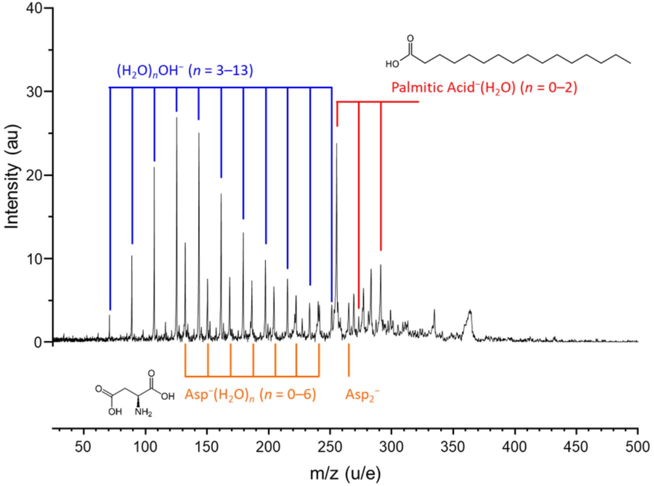
Results

Hypervelocity Ice Grain Setup (HIGS) at JPL

We have tested amino acids and fatty acids embedded within ice grains in HIGS, and demonstrated that we can accelerate them up to 5 km/s and record their mass spectra (below). We can also tailor the velocity distribution by varying the solvent ratio (right).

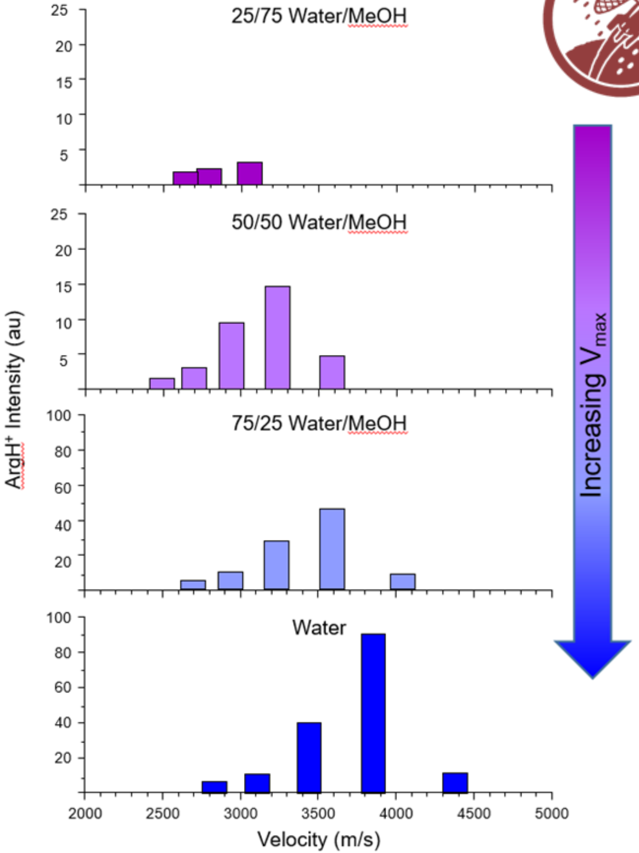
The next step is to impact these grains against a metal surface and determine how much of the biomolecules survive at different velocities. This will be done in the first quarter of FY21.



🟥 Fatty acid (palmitic acid)

🟧 Amino acid (aspartic acid)

🟦 Water and hydroxide clusters

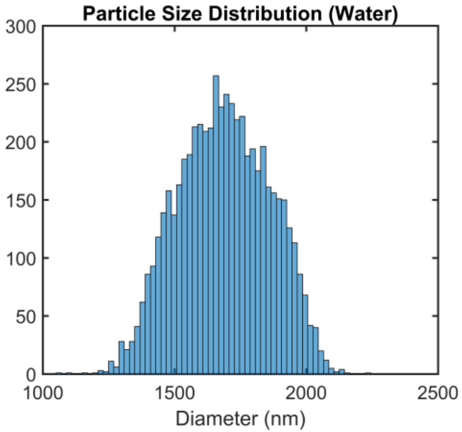


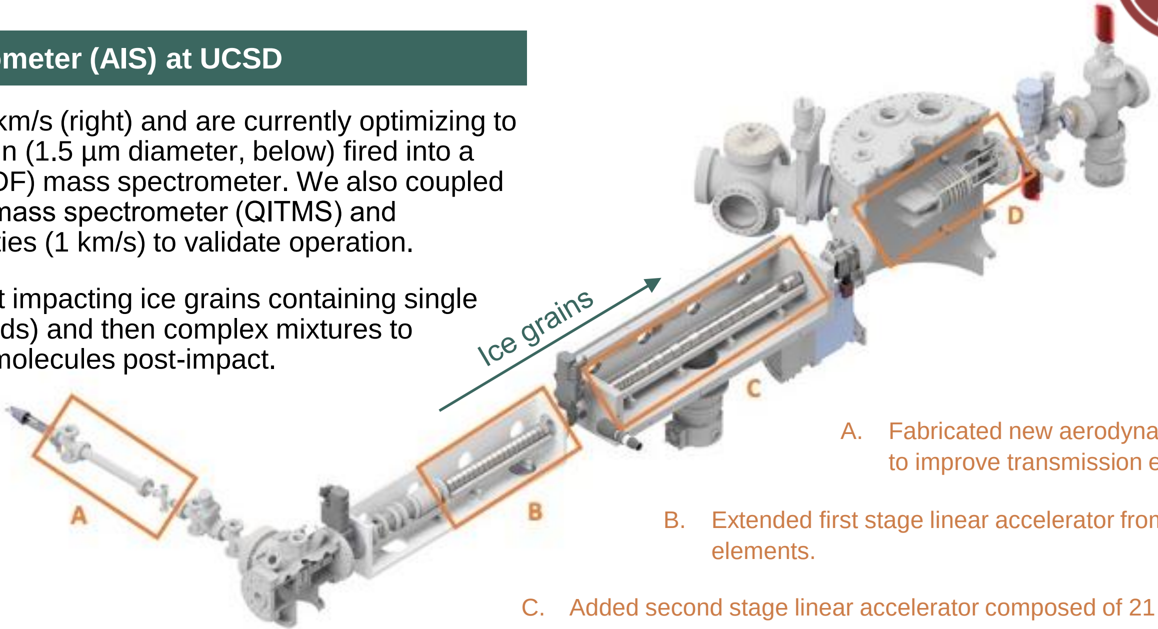
Results

Aerosol Impact Spectrometer (AIS) at UCSD

We have completed modifications to reach 5 km/s (right) and are currently optimizing to reach a new speed record for a single ice grain (1.5 µm diameter, below) fired into a target and measured using a time-of-flight (TOF) mass spectrometer. We also coupled this accelerator to JPL’s quadrupole ion trap mass spectrometer (QITMS) and performed test measurements at lower velocities (1 km/s) to validate operation.

The next step once we reach 5 km/s is to start impacting ice grains containing single biosignature molecules (amino acids, fatty acids) and then complex mixtures to determine if we can identify and quantify the molecules post-impact.





A. Fabricated new aerodynamic lens to improve transmission efficiency.

B. Extended first stage linear accelerator from 12 to 20 elements.

C. Added second stage linear accelerator composed of 21 elements, capable of accelerating 500 nm grains to 5 km/sec.

D. Fabricated and installed components for Time-of-Flight (TOF) Mass Spectrometer to measure single ice grain spectra after hypervelocity impact.

Pre-decisional: For Discussion Purposes Only

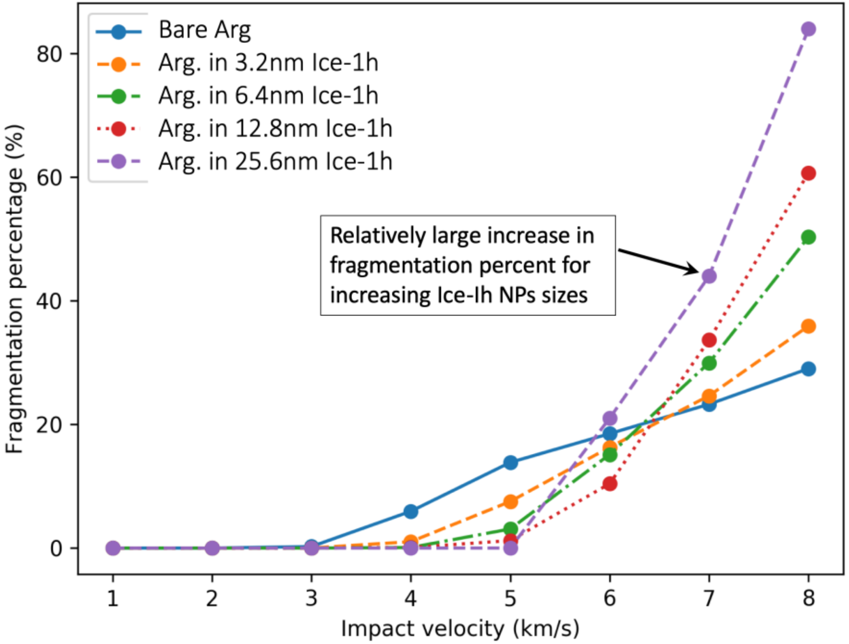
Results

Theoretical Modeling at Caltech

We have completed reactive molecular dynamics (RMD) simulations of impacts at 1-12 km/s for bare molecules (amino acids and fatty acids) and molecules embedded in ice grains up to 25.6 nm diameter (example for arginine at right). We have learned that these biomolecules do not necessarily break at the weakest bond, which is important to interpret mass spectra.

As expected, the ice shells dissipate impact energy and extend the velocity fragmentation threshold (the speed at which the molecules start to fragment). Predictions place ideal spacecraft encounter velocities between 3-5 km/s for bare amino and fatty acids and within 4-6 km/s for the same species encased in ice grains. A publication covering this work has been submitted to *Astrobiology* (in review).

The next step is to determine fragmentation dynamics and pathways for mixtures of amino acids and fatty acids to identify the optimal impact velocity range for Enceladus and Europa to minimize fragmentation and/or chemistry caused by impact.



Relatively large increase in fragmentation percent for increasing Ice-Ih NPs sizes

Summary

In just 2 years, we have built two experimental systems capable of accelerating ice grains to hypervelocity

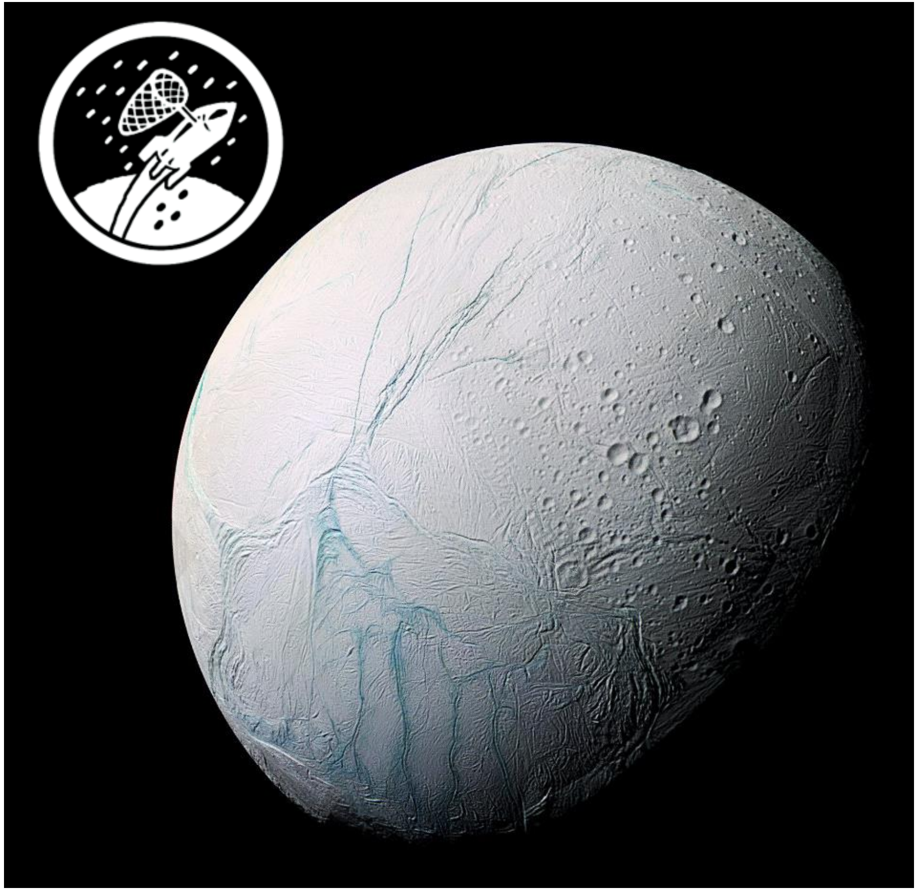
- Latest speed record for HIGS: 5.1 km/s (max of distribution)
- Latest speed record for AIS: 3.7 km/s (single ice grain)

We are at the forefront of theoretical modeling in this field

- Achieved successful reactive molecular dynamics simulation of impact of a 25.6 nm ice grain
- We can predict impact energy partitioning into vibrational, rotational and translational components
- We can predict mass spectra produced by impact-induced ionization

The infrastructure we have developed will enable instrument development for Ocean World life searches

- Both experimental systems can serve as testbeds for validating instruments that would sample a plume (Enceladus, Europa, comets)



Pre-decisional: For Discussion Purposes Only

Co-Is and Collaborators

JPL Co-Investigators

Name	Role	Section	Responsibility
Mike Malaska	Strat. Init. Lead	3227	Science vision; quarterly reviews; report submission including reviews.
Rob Hodyss	Co-I	3227	Advising on experimental design for ice grain experiments.
Amy Hofmann	Co-I	3227	Advising on experimental design and interpretation of complex MS spectra.
Sarah Waller	Co-I	353E	Lead for HIGS operation and experiments.
James Lambert	Co-I	389R	Evaluation of HIGS experimental design against requirements.
Anton Belousov	Co-I	389T	Integrating QITMS with AIS at UCSD. Characterizing impact of confounding species (isobars).
Stojan Madzunkov	Co-I	389T	Advising Co-I Belousov on QITMS experiments.
Nick Tallarida	Co-I	389R	Supporting HIGS experiments and data acquisition.

External Co-Is and Collaborators

Name	Role	Affiliation	Responsibility
Robert Continetti	Co-I	UC San Diego	Lead of AIS operation and experiments.
Andres Jaramillo-Botero	Co-I	Caltech (CCE)	Lead of theoretical modeling of ice grain impacts.
Jonathan Lunine	Collaborator	Cornell Univ.	Advising on interpretation of results and instrument performance reqs.
Bernd Abel	Collaborator	Univ. of Leipzig	Advising on HIGS operation and optimization.
John Eiler	Collaborator	Caltech	Advising on MS analysis and implications for mission architectures.
Hunter Waite	Collaborator	SwRI	Advising on implications of experiments for MASPEX.
Sascha Kempf	Collaborator	LASP	Advising on implications of experiments for SUDA.
Steve Fuerstenau	Collaborator	RadMet Inc.	Providing charge-sensitive detector (funded by SBIR).

Publications and Conference Proceedings

Conference Presentations and Proceedings

1. S.E. Waller et al. “Analyzing Enceladus’ Plume: First Steps to Experimentally Simulating Hypervelocity Impacts”, American Chemical Society (ACS) Spring 2020 National Meeting; Philadelphia, PA; March 21–26, 2020. (Oral)
2. A. Belousov, M. Miller et al. “Laboratory Simulations of Enceladus Plume for Flyby Mass Spectrometry Validation” Lunar and Planetary Science Conference; March 16-20, 2020.
3. A. Jaramillo-Botero et al. “Understanding hypervelocity sampling of ice-borne biosignatures in space missions.” AGU, Dec 2020. (submitted)
4. S. E. Waller et al. “Hypervelocity Sampling of the Enceladus Plume: Implications for Astrobiology Investigations” AGU, Dec 2020. (submitted)
5. S. Burke et al. “Characterization of the High Velocity Impact Phenomena of Small Water-Ice Particles” AGU, Dec 2020. (submitted)

Publications (completed or in preparation)

1. Jaramillo-Botero, A; Cable, M.; Hofmann, A; Malaska, R; Hodyss, R, Lunine, J. (2020) Understanding hypervelocity sampling in space missions. *Astrobiology*, in revision.
2. F. Klenner, et al. including M.L. Cable, R. Hodyss and J.I. Lunine (2020) Discriminating Abiotic and Biotic Fingerprints of Amino Acids and Fatty Acids in Ice Grains Relevant to Ocean Worlds, *Astrobiology*, ahead of print. https://doi.org/10.1089/ast.2019.2188
3. F. Klenner, et al. including M.L. Cable, (2020) Analog experiments for the identification of trace biosignatures in ice grains from extraterrestrial Ocean Worlds. *Astrobiology*, 20 (2), 179-189. https://doi.org/10.1089/ast.2019.2065
4. Cable, M. L. et al. “Plume Grain Sampling at Hypervelocity: Implications for Astrobiology Investigations.” White Paper submitted to Planetary Science Decadal Survey, 15 July 2020.
5. M.J. Malaska et al., “Membrane-spanning lipids as an agnostic biosignature.”In preparation. Targeting *Astrobiology*.
6. M. Miller, S. Burke, R. E. Continetti et al. Impact phenomena of Enceladus Ice Particle Analogs. In preparation.
7. Belousov, A. et al. Sampling Accelerated Micron Scale Ice Particles with a Quadrupole Ion Trap Mass Spectrometer. In preparation.