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Science Autonomy for Ocean Worlds Astrobiology: A Perspective

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Abstract

Astrobiology missions to ocean worlds in our solar system must overcome both scientific and technological challenges due to extreme temperature and radiation conditions, long communication times, and limited bandwidth. While such tools could not replace ground-based analysis by science and engineering teams, machine learning algorithms could enhance the science return of these missions through development of autonomous science capabilities. Examples of science autonomy include onboard data analysis and subsequent instrument optimization, data prioritization (for transmission), and real-time decision-making based on data analysis. Similar advances could be made to develop streamlined data processing software for rapid ground-based analyses. Here we discuss several ways machine learning and autonomy could be used for astrobiology missions, including landing site selection, prioritization and targeting of samples, classification of ''features'' (*e.g.,* proposed biosignatures) and novelties (uncharacterized, ''new'' features, which may be of most interest to agnostic astrobiological investigations), and data transmission. Key Words: Ocean worlds—Machine learning—Artificial intelligence—Neural network—Astrobiology. Astrobiology 22, 901–913.

1. Introduction

1.1. The need for science autonomy

Astrobiological discovery at an ocean world such as Enceladus or Europa will experience both scientific and technological challenges. The search for life and biosignatures deeper in the solar system faces enormous challenges for the supervision of science operations and planning. Here we discuss the technological obstacles associated with biosignature detection that are inherently intertwined with the agnostic detection of life; we focus specifically on the utility of autonomous operations in ocean worlds exploration, and how advanced data and computer science techniques, including machine learning (ML), could enhance astrobiologically relevant science data return and even enable new missions in these high-risk, high-reward environments. Missions to ocean worlds in particular are confronted with long communication delays (*e.g.,* 70–90 min between Earth and Titan), low bandwidth for data transmission, and potentially low power or energy supply, all of which decrease data transfer rates and volumes. In addition, missions to these targets will have protracted time intervals for data analysis and ground-in-the-loop, day-to-day decision-making (*e.g.,* ∼6 h between operational decisions, Europa lander: Pappalardo *et al.,* 2013; Hand *et al.,* 2017). Targets such as Europa have the additional challenge of an extreme radiation environment (Marion *et al.,* 2003), which will limit mission lifetimes and therefore the time to implement science-driven

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data collection strategies. All of these complicating factors strongly motivate development of more autonomous flight instruments and both onboard and ground-based software that can process data rapidly and consistently, streamlining science data analysis to maximize science return. This need has been recognized in the NASA Astrobiology Strategy (Hays *et al.,* 2015) and the National Academy of Sciences Astrobiology Strategy reports (National Academies of Sciences, Engineering, and Medicine, 2019) in findings that emphasize the necessity for new ML methods to explore large datasets and artificial intelligence applications that can autonomously conduct analyses.

Much of the mission autonomy development to date has focused on the onboard processing of raw data products that enables a spacecraft and/or flight instrument(s) to proceed safely and efficiently with mission objectives using minimal human interaction (Gao and Chien, 2017), which we term *robotic autonomy*. *B*y this definition, *robotic autonomy* would include automated navigation, instrument startup/standby/shutdown, and deployment of sampling mechanisms (*e.g.,* robotic arm movement, analysis chamber open/close). However, this definition of *robotic autonomy* is inherently linked with autonomous functions of instrumentation and data collection (*e.g.,* Ellery, 2018) and is the focus of this paper. For brevity and clarity, we refer to these capabilities as *science autonomy:* the ability of a science instrument to (1) analyze its own data in order to calibrate itself, (2) adjust and optimize operational parameters based on real-time findings, (3) prioritize data downlink, and (4) ultimately make mission-level decisions based on real-time scientific observations, including recommendations for subsequent analyses (*e.g.,* target selection, shifts in instrument mode such as narrow scanning ranges, or use of a different instrument). In this paper, we also use *science autonomy* to refer to Earth-based data processing software that could be used for rapid data interpretation by scientists. We recognize that *science autonomy* by these definitions is and will be integrated into further autonomous physical functions (*e.g., robotic autonomy*) and therefore exists as an intricate symbiotic relationship. We also offer a brief introduction on ML techniques tailored for the astrobiology and ocean worlds communities to better engage in future discussions of autonomy. Machine learning and artificial intelligence technologies could be used to the benefit of these communities to enable fundamental science by systematizing analyses toward an efficient search for canonical biosignatures, while also offering new agnostic insight to broaden the scope of astrobiological investigations (Conrad and Nealson, 2001; Chou *et al.,* 2021).

1.2. Autonomy-enabling algorithms: An introduction

Artificial intelligence (AI) has revolutionized the world in the past decades, encompassing any techniques that simulate human intelligence. As more sophisticated and powerful analytical instruments for astrobiology are developed and mission data are collected, the resulting increase in data volume necessitates advanced data analysis techniques that are able to process, interpret, and/or visualize the data at a rapid rate relative to manual processing by human investigators. Machine learning (ML) is a branch of AI that enables autonomous learning from datasets, trend/pattern identification based on real-time findings, and decision-making with minimal human intervention, and has become an integral tool in robotic space exploration. A computer system (an algorithm or program) can learn from data by first studying ''tasks'' and gaining ''experience,'' where the performance is measured, and the measured performance drives the algorithm to improve with experience (Mitchell, 1997). The goals of ML algorithms are to (1) receive input data, (2) use mathematical (*e.g.,* statistical) analysis to understand the data, and (3) fit that data into models in order to predict an output. Once the algorithm learns from the data, it is able to observe patterns in the data or make predictions about new and unknown data.

In this way, ML are algorithms that are able to compress cumbersome data volumes (with or without loss of information) for transmission, or identify and prioritize transmission of data with the most interesting or unusual characteristics (''novelty detection,'' Section 2.1.3). Some autonomy development uses ML to recognize patterns and develop predictive algorithms for data analysis or interpretation, while attempting to maintain the fidelity (low rate of error introduction) of the original data. There are several types of ML algorithms. **Supervised learning** algorithms are trained using input data that contains known information (labels); discussions with scientists and technologists about the structure, meaning, and importance of features of the input data are used to create ML labels. When using supervised learning algorithms, the dataset is split into a **training set** (a subset of the data used to train the model) and a **testing set** (a subset of the data, withheld during the training phase, used to test the model and assess its performances on unseen data). By comparing its results to the correct outputs, the algorithm modifies the model to minimize error and then learns from the process, allowing it to predict the correct output from input data based on the labels, and ultimately informing the predictions of new data without labels. However, supervised ML training efforts typically require large datasets (gigabytes to terabytes, depending on the technique and the problem); thus, their development for outer planet missions and astrobiology has received less attention due to the smaller data volumes expected. While small data volumes are riskier for ML training, efforts to use small datasets are expected to be more characteristic of ocean worlds and astrobiology missions. Fortunately, recent advances in data science have already begun to refine ML algorithms for smaller datasets (Li *et al.,* 2019). In comparison, **unsupervised learning** algorithms do not use labeled data as input; the user does not explicitly state known relationships between features in the data. The main goal of unsupervised learning algorithms is to explore and analyze the structure of the data in order to identify patterns and similarities (clustering) or to simplify the dataset (dimensionality reduction) without bias. Unsupervised learning algorithms are applicable when the phenomenon driving the data is unknown. Rather than making predictions about unknown data, the unsupervised algorithm makes a conclusion about the relationship within the data, allowing us to see patterns otherwise not recognizable by human investigators. Therefore, both supervised and unsupervised learning will be useful tools for future astrobiology missions.

Artificial neural networks (ANNs) are either supervised or unsupervised ML techniques that are inspired by the neurological structure of the human brain and aim to recognize underlying relations in a dataset by mimicking biological neural network (NN) processes. ML NNs are software algorithms that simulate neurons whereby interconnected neurons (the building block of a NN) are capable of processing information by dynamically responding to external inputs. In an ML NN, a neuron is ''a function''—a mathematical relationship from a set of inputs to a set of outputs—therefore, a NN is ''a network of functions,'' or an approximator of a larger function. A NN consists of several layers (Fig. 1): an input layer (containing the input data), an output layer (producing the predicted results), and one or multiple hidden layers within (determines relationships between input data). Layers are composed of nodes (neurons), and each node is connected to another node from the next layer with an assigned weight (relative importance / significance). More precisely, a neuron computes the weighted average of its input, which is then passed through a nonlinear function (called activation function) to generate an output. The output of a neuron can then be sent as input to another layer which will repeat the same process. Because this process can be performed using labeled or unlabeled data, the relative importance / significance of a particular input to the output can be evaluated using supervised or unsupervised ML. For a more detailed description of the mathematics used in ANNs, we direct the reader to several reviews (Knerr *et al.,* 1992; Kepka, 1994; Jain *et al.,* 1996; Bengio *et al.,* 2003; Basu *et al.,* 2010; Lazli and Boukadoum, 2013; LeCun *et al.,* 2015; Bala and Kumar, 2017; Abiodun *et al.,* 2019; Emmert-Streib *et al.,* 2020).

The primary task of a NN is to transform highly complex input into a meaningful output. A common analogy of a NN is that of a human brain processing visual data collected with their eyes. In this analogy, light is collected by the retinal array (input layer), which is then classified based on learned experience, including multiple steps involving processing the image data and extracting information (hidden layers). The brain then makes decisions about the surroundings by establishing a representation (output layer). While this example greatly simplifies the multitudes of complex processes associated with the analysis of visual data by the human brain, it serves as an intuitive analogy for applying ANN algorithms to astrobiological problems. For example, Storrie-Lombardi and Hoover (2004) investigated terrestrial fossils in astrobiologically relevant analog targets and classified them from their surrounding matrix using an ANN (Fig. 1). Compositional measurements collected on the fossil and surrounding matrix were pre-processed using principal component analysis (PCA), a dimensionality reduction technique, to determine which elemental abundances are most important in distinguishing between the matrix versus fossil material. These elements were used as input neurons/dataset for the ANN. The output predictions from this algorithm were then used to determine the original source of the samples (fossil versus matrix). The ANN was optimized by cross-referencing the ML predictions against classification done by a human expert or by comparing to the classes identified by the PCA. This type of ANN analysis helps provide a quantitative probabilistic methodology for spatially classifying biogenic versus abiotic materials.

Artificial neural networks can be more complex and composed of several hidden layers, such as in deep learning algorithms and autoencoders. Autoencoders have the advantage of having a simple ANN architecture, with several layers organized in a bottleneck. Autoencoders are ANNs capable of learning efficient representations of the input data without any supervision and are a form of data compression. Autoencoders, through an iterative training process, try to learn the features of a given input (for instance an image) and reconstruct the desired output (desired image) from these features. The two main tasks of an autoencoder are (1) to encode the input data into a condensed vector (called latent representation) and (2) to decode the condensed vector to restore the original data. Convolutional neural networks (CNNs) are a class of deep learning NN specialized in processing gridlike data (such as images or time-series data).

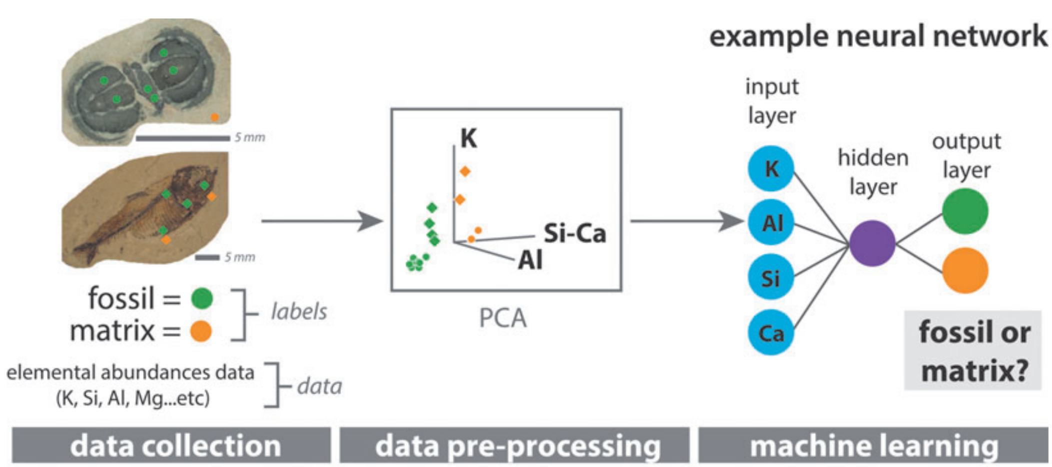

FIG. 1. Example workflow beginning with compositional analysis and data pre-processing of fossil versus matrix material in geologic samples. The raw data can be used as input for a neural network and machine learning algorithm training to autonomously distinguish and characterize fossil versus matrix material. Modified with permission from Storrie-Lombardi and Hoover (2004). Color images are available online.

Like NNs, CNNs are composed of different layers and can be described as the combination of two main building blocks: (1) the *convolution block* that enables the feature extraction of the data and (2) the *fully connected block* that performs the classification task. The main advantage is that the model learns an internal representation by extracting features from the input data and does not require engineered features from domain expertise. CNNs are commonly used in image processing and recognition. We refer the reader to several recent reviews of CNNs and deep learning (Aloysius and Geetha, 2017; Ajit *et al.,* 2020; Dhillon and Verma, 2020; Khan *et al.,* 2020; Alzubaidi *et al.,* 2021; Sony *et al.,* 2021).

As ML tools and predictive algorithms advance, mission concepts and science goals previously considered too risky or impossible due to data, time, or instrument power limitations can be explored (Azari *et al.,* 2021). Importantly, development of intelligent flight instruments will require accurate training datasets obtained from planetary analog environments, laboratory studies, and simulated data from model predictions, as well as rigorous testing of the algorithm(s) with an instrument of equivalent technology readiness level (Da Poian *et al.,* 2020) using *a priori* (prior) learning as a complement to onboard learning. A hybrid of these methods, in which ML algorithms are developed based on computational simulation and laboratory/planetary analog studies, would help predict, interpret, validate, and verify *in situ* measurements, and would be beneficial to science autonomy when availability of datasets is limited. The software development for an ''intelligent'' flight instrument necessitates a methodical evaluation process that can assess its critical function in not only executing the ML programs but also the hardware that will provide the computational power for the data processing. This can be achieved first on the ground (in the laboratory) and then in simulated, relevant space environments with mission constraints as would be expected on ocean worlds, which includes not only extreme temperatures and radiation but also limited bandwidth and data storage capacity and long communication times.

1.3. Onboard instrument autonomy

We consider two broad categories of science autonomy: flight instrument (onboard) autonomy and data interpretation autonomy. Onboard flight instrument autonomy deals with an instrument's ability to autonomously collect and selectively transmit data to Earth. Instruments capable of autonomous data collection, both robotically and in terms of decision-making (what samples to analyze, when, for how long, and fidelity of transmitted data) would, for example, greatly enhance the science return for missions with limited lifetimes due to extreme environments, and are being planned for missions such as the proposed Europa lander (Hand *et al.,* 2017). An increasingly important onboard autonomy consideration is that of data transmission; some flight investigations can generate far more raw data than can be downlinked to Earth; therefore, prioritizing downlinked data is a critical operation for future missions. For example, data volume for mass spectrometers has grown by orders of magnitude over the past decade (Guo, 2017; Da Poian *et al.,* 2020), while data transmission rates are expected to increase by at most one order of magnitude due to fundamental limits of physics (*e.g.,* antenna size and transmitter power limited by the spacecraft's mass, volume, and power or energy budgets). This difference between anticipated data volume and transmission implies that as much as 90% of the data generated by, for example, mass spectrometers on future missions—a potentially powerful life-detection technique—could not be transmitted to Earth.

1.4. Data interpretation autonomy

The second category of science autonomy focuses on data interpretation. Much of the mission data collected to date requires some level of processing and interpretation by individuals or working groups of engineers and scientists. However, such methods require significant personnel time and work efforts by one or more experts, which may not always be feasibly supported throughout the lifetime of a mission. These limitations can be overcome through the use of autonomous software able to make decisions depending on real-time observations/data. For example, the Autonomous Exploration for Gathering Increased Science (AEGIS) system uses ML algorithms to automate interpretation of visual images to assist in subsequent sample selection for the ChemCam instrument on board the Mars Science Laboratory (MSL) (Estlin *et al.,* 2014; Francis *et al.,* 2017), which has resulted in a significant increase in sampling and analysis. While data processing and analysis by experts is necessary for scientific advancement (and discoveries continue for years beyond a prime mission), science return would be enhanced by automating certain tasks such as initial reconnaissance for sample selection (Section 2.1).

Onboard instrument autonomy for sample selection and certain routine science measurement tasks (traditionally done by humans) could not only improve sampling cadence for remote and *in situ* planetary missions but also enable science activities in locations where explicit human direction is difficult or impossible. This capability will be necessary as missions extend deeper into the solar system and in extreme environments (*e.g.,* subsurface oceans), where data transfer rates are substantially outpaced by data volume generation rates, making supervision and planning of every analysis increasingly challenging. Beyond ocean worlds astrobiology, science autonomy could also open new capabilities for short-lived missions such as Venus surface investigation (as brief as a few hours) or atmospheric descent probes.

2. Science Autonomy Relevant to Ocean Worlds Astrobiology

In the following sections, we describe several critical needs for science autonomy for ocean worlds exploration, focusing on ways in which autonomous operations could be deployed on board a mission or during ground-in-the-loop evaluations to enhance astrobiologically relevant science data collection.

2.1. Sample target selection

2.1.1. Landing site selection. Currently, there are no established criteria for how to select a sample analysis site (≤ cm scale) for an astrobiology mission. Selection of a landing site (km scale) for *in situ* astrobiology seeks to mitigate engineering constraints (landing, mobility, and operations safety) while satisfying mission science goals. For example, the entry, descent, and landing (EDL) system for the Mars 2020 Perseverance rover autonomously selected and landed in a low topographic relief area of the Jezero Crater floor (engineering constraints) (Nelessen *et al.,* 2019), just east of an identified ancient river delta that is the focus of astrobiological science goals for the mission (Grant *et al.,* 2018; Farley *et al.,* 2020). Possible landing sites for the proposed Europa lander are Thera Macula or Conamara Chaos, both regions assumed to be recently disturbed due to the irregular icy blocks and reddish color characteristic of younger surface material on Europa (Fig. 2)

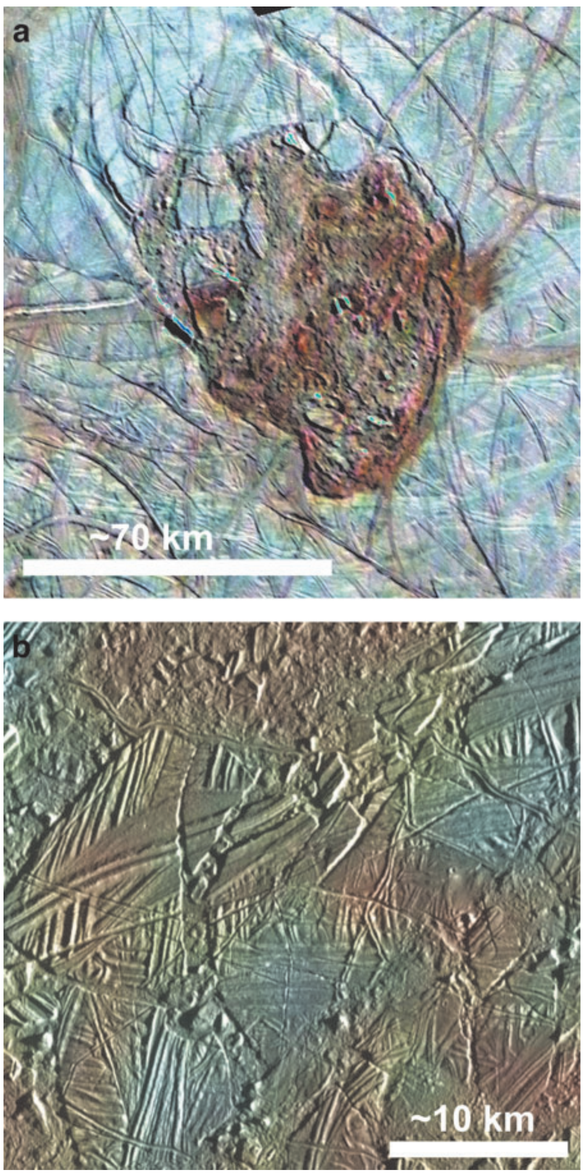

FIG. 2. (**a**) Thera Macula and (**b**) Conamara Chaos regions of Europa, both possible landing sites for an *in situ* Europa mission such as the proposed Europa lander, taken by the Galileo spacecraft. Red coloration is considered to indicate younger surface material on Europa (NASA/JPL/University of Arizona). Color images are available online.

(Schmidt *et al.,* 2011). Continued radiation exposure results in lighter coloration (Hand and Carlson, 2015; Schmidt, 2020). Either region's young surface could express material from the sub-ice ocean or intra-ice liquid pockets and therefore is considered an ideal surface target for astrobiology exploration (Kereszturi and Keszthelyi, 2013; Pappalardo *et al.,* 2013; Hand *et al.,* 2017). The proposed Europa lander intends to employ autonomous software similar to the EDL system used on MSL and Mars 2020 to identify surface characteristics (engineering constraints: *e.g.,* large blocks of ice, steep inclines) and autonomously choose a favorable site for landing. While EDL focuses on safe landing site selection, we suggest that similar Europa-specific technology could pair hazard identification with spectral imaging that uses the albedo of observed reddish-brown areas to indicate landing sites with more astrobiologically desirable sampling targets. In the case of Europa, the low-albedo chaos regions are indicative of younger salt-bearing surface material that has undergone limited irradiation, which would imply lesser degradation of possible biosignatures transported from the ocean below (Nordheim *et al.,* 2018).

In contrast, potential astrobiological missions to Enceladus focus on the collection of samples within and from fallout of Enceladus's plumes, which represent ''fresh'' material from the moon's interior oceans. The Enceladus Life Finder (ELF) and Enceladus Life Signatures and Habitability (ELSAH) mission concepts would sample the plumes directly during several flybys (Cable *et al.,* 2016; Eigenbrode *et al.,* 2018), while the Enceladus Orbilander mission concept would orbit before landing using autonomous terrain relative navigation (MacKenzie *et al.,* 2021). Sun *et al.* (2020) simulate various viffing (vector-in-forward flight) descents through Enceladus's plume(s) using lateral thrusters to maximize data collection about the plume while minimizing ΔV to deliver a penetrator spacecraft to Enceladus's surface, concluding that a biomimetic (quasi-spiral) search strategy would be the best candidate for development. Additional strategies, such as onboard plume source localization algorithms, are being explored to enhance targeting of Enceladus's vents through a sequential Monte Carlo method using a particle-based odor source localization technique (*e.g.,* Sun *et al.,* 2021).

2.1.2. Sampling target selection.

Once a spacecraft is landed and operational, the next challenge is to identify ideal sample targets ($\leq$ cm scale) within the reach of the spacecraft's sample handling system, which would include target identification, target access, sample collection, and sample processing. Of those capabilities, only the first—target identification—is separate from engineering and mission constraints. Astrobiological sample target selection is arguably the most challenging and subjective decision. This is due to a lack of consensus within the astrobiology community on what the most important/favorable features (*e.g.,* chemical or morphological) are for life detection in a location different from Earth. Even so, some reconnaissance spectroscopic studies could be automated and thus enhance target selection procedures. For example, on Earth, many biological entities express distinct spectral differences from their (abiotic) environment. Photosynthetic life produces biological pigments that absorb colors in the visible wavelength range (400–700 nm) (Seager *et al.,* 2005; Kiang *et al.,* 2007), and chemosynthetic microbes have shown a dynamic color range depending on nutrient availability (Brock and Freeze, 1969) (*e.g.,* the Grand Prismatic Spring, Yellowstone National Park, USA). Nonphotosynthetic pigments can also serve as biosignatures using spectral data (Schwieterman *et al.,* 2015). An observation of a spectrally interesting location could provide a compelling incentive to further explore the samples using chemical characterization techniques such as mass spectrometry. This approach may be complicated by extreme radiation environments (*e.g.,* Europa), which will necessitate sampling below the surface where organic material potentially deriving from life will be better shielded from radiolytic degradation (*e.g.,* >10 cm below surface: Hand *et al.,* 2017; Nordheim *et al.,* 2018).

Visual characteristics ideal for astrobiology will likely be specific to a planetary target, and therefore a combination of nondestructive techniques may be the most robust method for selecting samples for follow-on destructive sample analysis. Nondestructive techniques may have specific sample requirements (*e.g.,* surface characteristics, albedo, sample type [solid / liquid or rocky / icy]); therefore, a targeting procedure could be implemented based on a list of requirements. For example, the Scanning Habitable Environments with Raman and Luminescence for Organics and Chemicals (SHERLOC) instrument on board the Mars 2020 Perseverance rover is characterizing organic matter and minerals on the martian surface to evaluate habitability markers, prebiotic chemistry, and potential biosignatures. SHERLOC includes an Autofocusing and Contextual Imaging (ACI) subsystem that provides image z-stacks, which feeds into a macro mapping mode and autonomous micro mapping mode, triggered by either greatest signal intensity or specific spectral features, and may include point spectra (Beegle *et al.,* 2015). Such nondestructive techniques, which are also under development for ocean worlds and Venus missions (Wang *et al.,* 2015; Tallarida *et al.,* 2018), could serve to triage high-priority samples for more invasive analytical techniques such as laser desorption mass spectrometry (LDMS).

2.1.3. Relevant machine learning applications. While not exhaustive, in this section we highlight some ML techniques that may be utilized for automated sample site characterization and sample targeting for subsequent chemical/morphological analyses. We classify two broad qualities, termed novelty and feature detection, that could be characterized by ML and autonomously detected in a planetary environment, and how these qualifications relate to life detection.

Novelty detection. Data mining techniques such as novelty detection—the identification of novel (new) or unobserved data that an ML system has not seen during its training (Miljković, 2010)—can be used in the identification of targets. Novel features can be categorized as those that (1) are well documented but are known to occur rarely, (2) have not been detected before, (3) are not expected (*i.e.,* an outlier in the given setting), or (4) appear different from previously seen features of the same type. Known novelties (*i.e.,* those from categories 1, 3, and 4) are usually studied using a supervised learning approach designed to classify these novelties with only a few training examples. The model learns to identify the class that is underrepresented in the training data by leveraging some combination of learning from well-represented classes (Bart and Ullman, 2005; Vinyals *et al.,* 2016), leveraging external semantic information (Wang *et al.,* 2017), or simulating more examples of the novel classes with which it can then train on (Fei-Fei *et al.,* 2006). Since this is a data-intensive activity and the available data from ocean worlds environments are sparse and low-resolution, early ML algorithms may be trained using data available on Earth; then that knowledge would be ''transferred'' (or applied) to a new environment, termed transfer learning. Transfer learning leverages developed algorithms on large datasets from relatively similar data in order to adapt algorithms to more limited analog environment training data. For example, a representation of basaltic rocks could be learned by using feature representations of terrestrial basaltic rocks, expected structural/mineralogical characteristics, or a quantity of simulated basaltic outcrop examples in order to identify basaltic features on, for example, the Moon or Mars.

In contrast, the lack of definition and examples of the novelty class for unknown novelties (*i.e.,* category 2) requires an unsupervised learning approach. Previous work has shown promising results in using autoencoder networks to detect novel observations and sensor readings (Hinton, 2006; Xiong and Zuo, 2016; Richter and Roy, 2017; Raimalwala *et al.,* 2020; Stefanuk *et al.,* 2020). Recent work by Kerner *et al.* (2019, 2020) has demonstrated the capability to detect novel geological features in multispectral images of the martian surface using autoencoder approaches. They also compared several methods on the multispectral dataset—Reed Xiaoli (RX) detectors, principal component analysis (PCA), generative adversarial networks (GANs), and autoencoders—and show that (1) the RX and autoencoders trained with structural similarity loss are able to detect novelties based on morphological features, which are not detected by other methods, (2) PCA and GANs are better suited for detecting spectral-feature novelties, and (3) autoencoders provide the most useful way to visualize the detection of novel features.

Feature detection. Beyond the detection of novel features, it is also important to characterize the known and commonly occurring features in the environment observed by imagers or spectrometers. A widely used technique in Earth science, now being used on Mars (Francis *et al.,* 2017) and developed for the Moon (Raimalwala *et al.,* 2020), is CNNs that classify natural features and complex patterns in an image (Fig. 3). This classification is performed using supervised learning, in which, for example, the features in a terrain image are labeled in minute detail to create a deep learning (*e.g.,* CNN) model of terrain that is representative of a mission's environment. Features classified from multiple images can be aggregated to construct a rich representation of the surrounding environment and provide geologic context, which can be used by other software applications to make decisions on prioritizing targeting or downlink of instrument measurements. While missions to Mars have collected sufficient data for such modeling using years of chemical (ChemCam, MSL) and high-resolution imaging (HiRISE, MRO) data, an ocean worlds mission could use

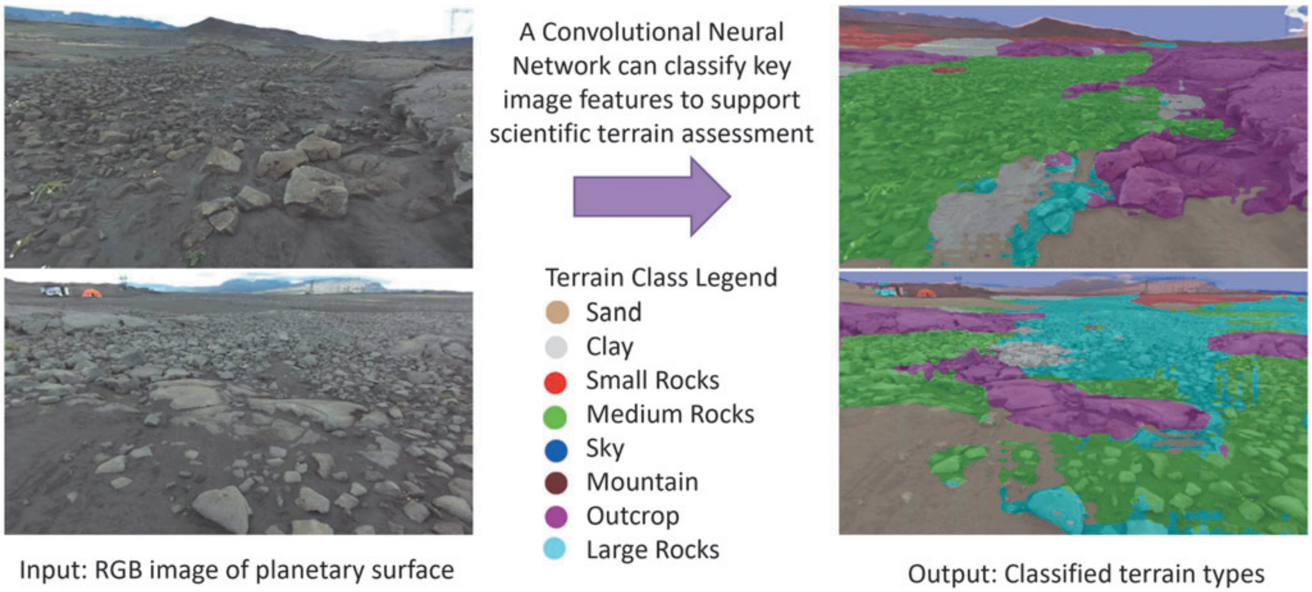

FIG. 3. Example of terrain classification using a deep learning technology developed by Mission Control (Raimalwala *et al.,* 2020). Rover-based images from a Mars 2020 analog research study in Iceland were segmented into Mars-relevant terrain classes to support scientific terrain assessment as part of SAND-E (Semi-Autonomous Navigation for Detrital Environments). Color images are available online.

models trained on data from a high-fidelity analog environment such as Antarctic and Arctic sea ice, and use transfer learning techniques to adapt algorithms to laboratory simulation datasets that include extreme gravitational, thermal, pressure, and radiative conditions.

While the above techniques are powerful tools to rapidly evaluate surface characteristics and select a target for analysis, beyond a visual detection of a life-form, datasets such as mass spectra may be more likely analyzed in search for potential biosignatures (*e.g.,* complex biological molecules or molecular fossils); and analytical methods for tandem mass spectrometry (MS/MS) such as the kinetic method, chiral recognition ratio method, and photodissociation mass spectrometry method, or ion mobility mass spectrometry have shown promise for measuring enantiomeric excess and chiral differentiation (Han and Yao, 2020). During a mission, ice and/or mineral samples would be collected, potentially triaged by nondestructive methods (as described above), and transferred to a mass spectrometer for detailed analysis. In particular, features such as complex organic molecules (Marshall *et al.,* 2017, 2021), enantiomeric excess of chiral organic molecules (Glavin *et al.,* 2020), and large observed isotopic fractionations (*e.g.,* tens of per mil (‰) in $\delta^{13}C$) are considered potentially powerful indicators of life (Hayes, 2001). Ongoing efforts in mass spectrometry analysis for astrobiology have also shifted focus from searching for organic biosignatures indicative of Terran-based life (Summons *et al.,* 2008) to those that may be based on unfamiliar biochemistry (*i.e.,* life as we don't know it, or ''agnostic biosignatures'') (Conrad and Nealson, 2001; Johnson *et al.,* 2018; Chou *et al.,* 2021). Several types of onboard autonomy should enhance our ability to identify the most characteristic or unique spectra for further analysis, as discussed in the next three sections.

2.2. Critical evaluation of calibration data

Regardless of the specific environment (laboratory vs. planetary surface), instruments routinely go through a calibration sequence before and/or after characterizing unknown samples to achieve maximum, for example, ion transmission, signal reproducibility, and/or quantitative accuracy depending on the main science objective. Calibration typically involves analyzing one or more reference materials and tuning any number of adjustable instrument parameters, such as gas flow rates, filament current settings, and voltages or timing delays applied to active electrodes, while maintaining baseline performance metrics. Thus, real-time validation of data quality is a prime candidate for onboard science autonomy.

Data derived from the analysis of well-characterized reference materials are the most common products generated by instruments. Reference materials facilitate tracking of instrument performance as a function of time and also as spaceflight integration and testing progresses; they also provide a reference by which to compare subsystem functionality during tuning and troubleshooting stages. Therefore, most instruments have an abundance of high and low quality calibration data (*e.g.,* sensitivity, accuracy/precision). These volumes of calibration data are ideal for training and validating ML algorithms. If an instrument performs a ''good'' calibration—however such a pass/fail criterion may be defined—the onboard software will authorize the analysis of unknown samples without needing ground-in-the-loop human interactions. Such calibration data could be stored and transmitted at a later time so that the data sent back first are preferentially from samples, enhancing data economy (the effective cost per byte of science data), the utilization of onboard resources, and ultimately the prioritization of science return. This approach is currently in development by the

Mars Organic Molecule Analyser (MOMA) science and engineering team, which seeks to design ML-based software that is able to discriminate calibration mass spectra from mass spectra obtained from the analysis of planetary analog samples (Da Poian *et al.,* 2020). More progressive autonomous decisions could enable advanced calibration techniques for more focused investigations, such as instrument tuning that maximizes mass spectrometric ion transmission within a narrow mass range for isotopic studies, or *in situ* troubleshooting in response to degrading calibration data quality.

2.3. Discrimination of data at a threshold

Once an instrument has begun data collection on an unknown sample, the next opportunity for autonomous decision-making is the discrimination of high-priority data, such as those above the threshold of a limit of detection (LOD), those that display unique or diagnostic patterns, and those that corroborate observations collected by other payload instruments. Various routine data pre-processing techniques may be employed prior to data triage: background removal via polynomial fits, stacking of multiple spectra, noise detection via deep learning NNs, and so on. These methods enhance signal-to-noise ratios of raw data, enable automatic determination of LODs, and assist the selection of high-quality data for subsequent qualitative and/or quantitative interpretation. For example, if a mass spectrometer has an LOD of 20 ppbw for glycine, any pre-processed data collected that indicate ≤20 ppbw glycine in the sample would be considered low priority using that metric alone. The instrumental response to background signals and/or calibration analytes can be used to infer quantitative information. A possible use of such information could have been the detection of molecular hydrogen (H_2) in Enceladus's plume by the Ion and Neutral Mass Spectrometer (INMS) on board the Cassini spacecraft. Waite *et al.* (2017) demonstrate the detection of H_2 above background $+3\sigma$, which combined with the detection of silica particles in the plume (Hsu *et al.,* 2015) suggests hydrothermal activity at the interface of the subsurface ocean and rocky core. Subsequent comparison of data across multiple analytical runs and/or instrumental suites could prioritize features of interest with high reproducibility above the established LOD (*e.g.,* background $+3\sigma$). An astrobiological example might include prioritizing spectra that exhibit a broad range of high carbon number molecules above a specified LOD, or above the limit of quantitation (*e.g.,* background $+10\sigma$) for more rigorous statistical analysis.

Diagnostic patterns and/or features in datasets can also provide qualitative assessments of raw data, which can be characterized via pre-trained ML algorithms or using an exploratory approach. For instance, ML classifiers that pretrained on terrestrial rock images achieved 100% accuracy in the classification of martian lithologies observed in high-resolution images collected by the Curiosity rover (Li *et al.,* 2020). Mass spectra of different organic compounds such as lipids, proteins, and aromatic hydrocarbons show characteristic peak distribution patterns. Therefore, spectral information such as mass range, number of peaks, and relative abundances are useful variables to evaluate the presence of complex molecules and classify their molecular classes (Guttenberg *et al.,* 2021). Data obtained from multiple measurements could be compressed using dimensionality reduction methods (*e.g.,* PCA), summarized using statistical analysis (*e.g.,* average and standard deviation), or simplified using sum-averages of similar measurements to reduce the volume requirements for data transmission. Prioritizing which data to send back first based on the transmission constraints (*i.e.,* transmission rates and data volume) could be critically accomplished based on signal intensities, features, and/or patterns observed above using a decision tree, a weighted scoring system of multiple criteria, or statistical analysis to assist system-level or mission-level decision-making. We present an ocean-worlds relevant example of this workflow for Orbitrap mass spectrometry analysis in Section 2.4.

2.4. Novelty and feature detection

Following the detection of a novelty or feature (Section 2.1.3) (*e.g.,* the detection of one or more peaks above the LOD within a targeted mass range), the data can be either preferentially sent back first for ground-based analysis or processed further using onboard software to determine composition or inform on follow-up experimental procedures. A fast and preliminary analysis is encouraged for onboard data processing in order to isolate low-priority data without further analysis. Quick assessments of data can provide timely instructions to tune instruments for subsequent measurements in order to collect a more optimized signal. For example, absence of peaks in mass spectra can be made to autonomously trigger output energy of an LDMS laser source to enhance multiphoton ionization, based on a systematic ML of ionization responses. In addition, more extensive onboard data processing would provide an opportunity for ground-based scientists and technologists to make critical decisions about how to conduct follow-up experiments based on real-time data interpretation. For example, MS/MS techniques could be applied to prospective macromolecular complexes detected with sufficient ion intensity by the MOMA instrument in order to elucidate structural information (Goesmann *et al.,* 2017). Because MS/MS requires the selection of which ions of interest are the most compelling to fragment, autonomous software could effectively circumvent the need to involve ground-based (human) decision-making and lose valuable time. The essence of autonomous decision-making is to select an action that maximizes science return while minimizing associated risks for subsequent implementation. Without knowing what could happen next, a decision computation model (such as those built on Markov decision processes or recurrent neural nets) must balance between the scientific gain when a specific ion of interest is chosen to perform MS/MS and the cost (*e.g.,* data volume and time) when additional measurements are taken. This onboard autonomy would therefore enable ground-based scientists to focus on analysis of optimized science data.

Moreover, information sharing between instruments can also facilitate data collection for the greatest science return. Prompted classification and interpretation of data collected from non-invasive techniques, such as imaging or high-resolution spectroscopy, can critically assess the textural and/or chemical heterogeneity of environments and targeted samples (Section 2.1.2). Such information can inform subsequent measurements, such as mass spectrometry or X-ray fluorescence spectroscopy, about the location of highly interesting areas or the number and distribution of measurements needed to obtain spatially representative results.

When using or developing multiple data processing procedures, a workflow can be tailor-made to streamline data collection, data processing, and onboard instrument payload coordination. An example of an AI data processing workflow proposed to handle time-series data generated from the Characterization of Ocean Residues and Life Signatures (CORALS) Orbitrap mass spectrometer is shown in Fig. 4. Data processing of transient spectra recorded by CORALS could not only be able to identify the stoichiometry of molecules via exact mass measurements but also simultaneously derive collision cross-sections to elucidate molecular structures, and inform subsequent scans with narrower mass ranges to improve local dynamic range and quantify isotopic abundances (Arevalo *et al.,* 2018; Willhite *et al.,* 2021). Such progressive analyses and data processing may require additional resources (*e.g.,* power, energy, data volume) but could maximize the useful information per byte of missions with limited lifetimes and constrained communications, such as the proposed Europa lander mission.

Autonomous data analysis is currently in progress by several research groups, yet the current algorithms developed to our knowledge have focused primarily on discrimination of calibration data and data below threshold criteria (Sections 2.2 and 2.3), as well as data compression techniques for downlink (Section 2.5) (Reeder and Gough, 1996; Da Poian *et al.,* 2021; Xie *et al.,* 2021). Developing ML algorithms for astrobiological use is further complicated by novel features such as agnostic biosignatures, that demonstrate the inherent complexity of organic compounds (*e.g.,* biopolymers), elemental and isotopic abundance patterns in assemblages of compounds and mineral phases, morphological features (*e.g.,* concretions or biomats), surface complexity (*e.g.,* abundant surface expressions on cells vs. simple mineral faces), and sequestration of certain elements in cells that are reflective of biological activity rather than abiotic sources (*e.g.,* Williams and Da Silva, 2000; Slaveykova *et al.,* 2009; Kempes *et al.,* 2016; Marshall *et al.,* 2017; Johnson *et al.,* 2018; Neveu *et al.,* 2018; Chan *et al.,* 2019; Pohorille and Sokolowska, 2020; Kempes *et al.,* 2021; Marshall *et al.,* 2021). Thus, access to as many different classes of prospective biosignatures as possible, commonly referred to as orthogonal detection, is a major objective of next-generation payloads to increase confidence in findings and avoid false positives. Autonomous data analysis and onboard command tools hold the promise to categorically rank broadband spectra and determine which samples warrant more focused investigation without waiting for ground-based decisions.

As an example, the Europa Lander Science Definition Team report (Hand *et al.,* 2017) indicates that ''sample acquisition is anticipated to last 5 hours'' and ''the science and engineering teams have 8 and 16 hours, respectively, to plan and generate commands for the subsequent [24 hrs], which includes making the decision on the activities for the next [24 hrs].'' A single Earth day could result in $\sim$70 Mb of raw, unprocessed data, transmitting at a rate of 80 kbps that would need to be processed and analyzed before science and engineering teams could make operational decisions and send updated commands. The short mission duration (20+ days per the baseline scenario), abbreviated analysis times as described above, and large data volumes generated necessitate the development and deployment of science autonomy to maximize science return. Such autonomous

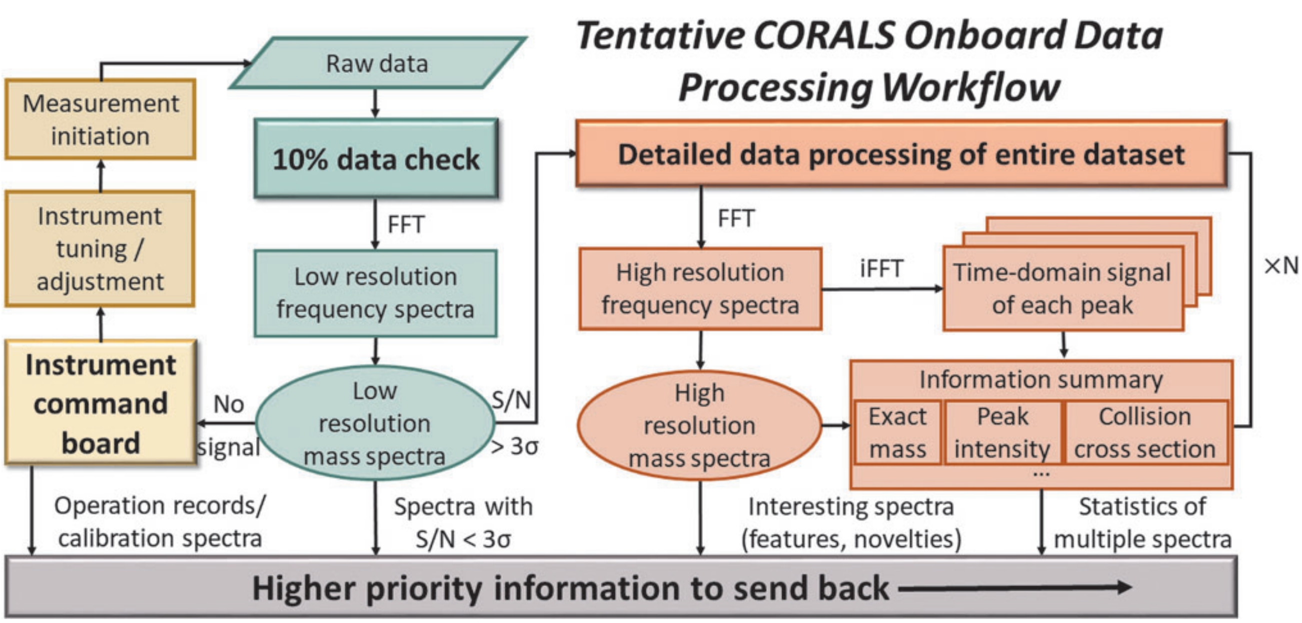

FIG. 4. A provisional CORALS Orbitrap mass spectrometer onboard data processing workflow composed of four interconnected sections: instrumental responses and data collection (yellow), preliminary/quick analysis (green), more detailed onboard data processing (orange), and a proposed priority ladder for deciding which data should be sent back (gray). Bold text highlights the four primary steps for onboard data processing. The communication between these four sections streamlines data collection and processing, adjusts instrumental parameters autonomously to reach maximum performance, and critically evaluates the priority of data products for return transmission. FFT = fast Fourier transform. S/N = signal-to-noise ratio. Color images are available online.

applications would also be highly important for the Dragonfly mission scheduled to launch to Titan by 2027. In particular, the Dragonfly Mass Spectrometer (DraMS), a payload investigation on board the Dragonfly octocopter, comprises heritage subsystems derived from the Sample Analysis at Mars (SAM) and MOMA instruments (Lorenz *et al.,* 2018). Like MOMA, DraMS will be capable of MS/MS, allowing for controlled fragmentation of molecular species to provide robust structural analysis of highly complex molecules. Given the vast distance between Earth and Titan, the light travel time naturally inhibits the quick downlink of data to be processed and peaks to be chosen for fragmentation by ground-based personnel. Therefore, the development of autonomous software is highly advantageous to select feature or novelty peaks based on ML algorithms that were trained on calibration data during integration and test activities, chemical data collected from laboratory simulants of Titan's atmosphere, or newly collected data derived from the *in situ* analysis of samples on the surface of Titan.

2.5. Data transmission and downlink

An additional complication that could be mitigated using ML is in managing how data is transmitted to Earth, whereby the volume of collected data often exceeds the transmission rate. While missions closer to Earth do not experience the same strain on the ability to transmit data (and receive commands), data of astrobiological significance (*e.g.,* fluorescence, mass spectrometry, Raman spectroscopy, microscopy) collected during outer solar system ocean worlds missions will inevitably outpace the capacity to transmit back to Earth. Two current strategies for reducing transmission volumes are compression and segmentation. Autoencoders are popular ML algorithms for data compression that can also be used to reduce dimensionality in a dataset. An autoencoder stacks multiple nonlinear transformations that can model complex functions, whereas PCA (a widely used tool in dimensionality reduction) only uses single linear transformation. The PCA transformation maps data as orthogonal vectors in multidimensional space where the axes (also called ''principal components'') represent the maximal amount of variance in the dataset (*e.g.,* the directions capturing the most information of the data). An autoencoder, on the other hand, maps (encodes) input to a latent space with reduced (compressed) dimension but has been trained to faithfully reconstruct (decode) input. Data with high dimensionality (*i.e.,* images) can be projected or encoded into lower-dimension representations, which can then be recovered using a pre-trained decoder network without significant information loss. Training of a high-performance autoencoder, however, requires large synthetic or empirical datasets. Segmentation, on the other hand, simplifies the representation of multidimension datasets into groups or clusters of similar characteristics, yet omission of details may induce information loss. Both techniques could reduce data volume, but high compression ratios can introduce severe artifacts. Subtle features in spectra can be lost, and if the most important or valued measurements are only a small fraction of the total data collected, then compressing and preserving the whole population is often done at the expense of the vital subpopulation. Thus, autoencoders and segmentation (using an algorithm to separate out a key segment or subset of data) require schemes that reliably do not remove critical data.

As an example, a preliminary concept of operations from the ultrahigh resolution CORALS mass spectrometer projects >5 Gb of data volume produced per analyzed sample (with no data compression). With the CORALS instrument, a high-resolution mass spectrum (*i.e.,* $m/\Delta m > 100{,}000$ at mass 100) requires a transient of approximately 840 ms (Briois *et al.,* 2016), equating to 2^{22} (or $\sim 4 \times 10^{6}$) data points at a sampling rate of 5 MHz. The number of data points doubles if $1\times$zero filling is applied, a common practice for digital signal processing that serves to increase frequency resolution. Assuming 16-bit vertical resolution, a fast Fourier transform that includes both real and imaginary components comprises 2^{27} bits; however, the standard CORALS data processing routine generates magnitude-mode frequency spectra, thereby reducing the data volume of a single analysis to 2^{26} bits (or ~ 67 Mb). The CORALS laser system is capable of actively scanning across the surface of a sample within a 500 μm diameter field-of-view, enabling 2D chemical mapping. An elliptical laser beam footprint with a minor diameter of 50 μm (due to a 45° angle of incidence) at the sample surface results in a chemical image with approximately 36 resolved ''pixels,'' multiplying the data volume accordingly. Because repeated analyses are essential to building statistical confidence and reducing the risk for false positives (particularly for life-detection missions, *e.g.,* Neveu *et al.,* 2018), triplicate measurements at each image pixel would result in a $>100\times$ increase in the data volume for a single sample. Therefore, after accounting for per-pixel sampling and replicate analysis, the single sample uncompressed data volume from the CORALS instrument can easily exceed 5 Gb.

Due to limited downlink data rates (*e.g.,* Hand *et al.,* 2017) and the large data volume of the CORALS instrument, each sample spectrum would require substantial data reduction, pre-processing, and compression before transmitting to Earth. Data compression could result in substantial reduction of the data quality and mass resolution, each of which are critical features of the CORALS design. Therefore, any loss in data quality due to compression negates the significant analytical advantage of the CORALS instrument over lower-resolution mass spectrometers. Thus, it is important to implement a balanced approach when using data compression and segmentation, especially to preserve critical information in high-resolution data such as those enabled by CORALS. Likewise, developing, testing, and validating this functionality during instrument development would significantly improve onboard autonomy capabilities.

3. Concluding Remarks

New frontiers of scientific and specifically astrobiological exploration bring about new challenges. As we broaden our search for life elsewhere in the outer solar system's ocean worlds, our technological and scientific knowledge must also advance to meet the requirements necessary to qualify a sampling campaign as a life-detection event. In addition to the well-known mechanical and operational challenges associated with exploring deep space, there are also constraints posed by data collection and transmission, or even mission lifetime (*e.g.,* Europa and Venus). Many missions have severe limitations on the volume of data that can be transmitted, requiring innovative new strategies to optimize data collection and prioritization. This is particularly important since life detection requires multiple lines of evidence, from various instrument platforms, and within a thoroughly investigated environmental context—a feat which requires high volumes and diversity of data. Fortunately, there are methods that go beyond the classical compression and data partitioning schemes; novel ML methods can form the basis of an onboard data budget by making informed decisions based on real-time data collection and autonomous analysis. Science autonomy can also triage targets and collected data. The key challenges of data collection and transmission are ideally addressed in concert, as they are not fully separable problems. They require us to use all the knowledge we have from prior studies, particularly in astrobiologically relevant Earth-based planetary analogs, as well as an assessment of all the potential characteristics of the environment to be studied. Investment in, and development of, science autonomy capabilities expands our astrobiology discovery capabilities; in some cases, it allows us to access new scientific information and explore frontiers that would not be possible otherwise. A successful science autonomy strategy requires investment and development to ensure that the methods are robust and reliable. Doing so ensures that state-of-the-art methods are infused into the mission cycle, traceable from science objectives all the way to mission operations and data interpretation, so that we can take full advantage of exciting new frontiers of exploration.

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Abbreviations Used

AI = artificial intelligence
ANNs = artificial neural networks
CNNs = convolutional neural networks
CORALS = Characterization of Ocean Residues and Life Signatures
DraMS = Dragonfly Mass Spectrometer
EDL = entry, descent, and landing
GANs = generative adversarial networks
LDMS = laser desorption mass spectrometry
LOD = limit of detection
ML = machine learning
MOMA = Mars Organic Molecule Analyser
MSL = Mars Science Laboratory
MS/MS = tandem mass spectrometry
NN = neural network
PCA = principal component analysis
RX = Reed Xiaoli
SHERLOC = Scanning Habitable Environments with Raman and Luminescence for Organics and Chemicals