The following gap list is a result of the precursor science workshops, “Precursors to Pathways: Science Enabling NASA Astrophysics Future Great Observatories”, that occurred in April and October 2022. The workshops’ goal was to foster discussions that will inform the creation of a gap list that would identify needed investigations that would help define the performance and architectures of the observatories. The workshop also provided opportunities for community members to engage with each other and NASA on potential ideas for precursor science investigations in preparation for submitting proposals and thus providing a list of science investigations that can be significantly impactful on the mission architecture in areas such as these:

- Modeling of target spectra, and the needed laboratory astrophysics measurements needed to support such modeling, that would better define the sensitivity, spectral resolution, and wavelength coverage needed to detect key atomic/molecular/ionic species relevant to the mission's main science goals.

- Improved constraints on the occurrence frequency of key science targets that must be observed in order to achieve the mission's main science goals, in order to better understand the scope of surveys that must be carried out by each mission to capture those targets. Identification of specific key science targets in advance, if this would significantly improve the efficiency of such surveys.

- Modeling or observations of background levels and background source counts that can confuse or limit detections of key targets that must be observed as part of mission main science goals.

- Development of mission simulation software that improves the fidelity of throughput and yield calculations, and helps develop operations scenarios, in order to better constrain the mission time needed to conduct key projects as well as the overall mission lifetime requirement.

- Development of quantitative science metrics that should be used to evaluate the ability of mission architecture options to achieve the mission's main science goals.

Table of Contents

#1 Modeling Exoplanet Atmospheres and Biosignatures

<u>Gap Summary:</u> Spectral modeling is essential for inferring the properties of exoplanet atmospheres from observations.

<u>Relevance to Mission Architecture:</u> Modeling informs the spectral resolution, wavelength coverage, and signal to noise ratios needed for IROUV instrumentation that will measure critical diagnostics of exoplanet atmospheres. It is especially important for anticipating the observed properties of exoplanets that are unlike those in our own solar system.

<u>Capability Needed:</u> Ability to model the physical and chemical structure of exoplanet atmospheres and their emergent spectra across the range of planet masses, sizes, and stellar host types. Treat the effects of the total atmospheric pressure; chemical composition; presence of condensates, clouds & hazes; observer phase angle; and the radiative and energetic particle fluxes incident from the host star. Understand how the exchange of matter and energy between exospheres, lithospheres, hydrospheres, and potentially biospheres affect the observed properties of the atmosphere today and over the planet's history.

<u>Capability Today:</u> Thermophysical, radiative transfer, and photochemical models of planetary atmospheres in the solar system. Modeling of brown dwarf and hot giant exoplanet spectra including the effects of non-uniform cloud cover, atmospheric chemistry, and radiation-driven atmospheric escape. Biosignatures and their false positives have been explored (e.g. June 2018 special issue of *Astrobiology*)].

#2 Precursor Observations of IROUV Exoplanet Imaging Targets

Gap Summary:. Improve knowledge of plausible IROUV target star systems to firm up the stellar properties and determine whether their habitable zones are free of potential confusion, are dynamically stable, and what levels of ionizing radiation are present.

Relevance to Mission Architecture:
Improved knowledge of plausible IROUV target stars can improve the fidelity of exoplanet yields estimates used for architecture trades. If a significant fraction of nominal IROUV targets are compromised, then changes to the telescope aperture and/or starlight suppression requirements may be needed to increase the number of accessible "clean" target systems.

Capability Needed:
A census and characterization of plausible IROUV target systems, including their stellar and substellar companions which may dynamically limit the presence of planets in their habitable zones. Theoretical research constraining the stability of planets in their habitable zones. Sufficiently sensitive X-ray and far-UV characterization of stellar radiation environments in the target systems.

Capability Today: The census of even massive companions (low-mass stars, brown dwarfs, giant planets) is still incomplete for plausible IROUV targets. The HabEx and LUVOIR teams conducted yield simulations based on the Hipparcos star catalog with very limited binary star info and initial estimates of key stellar astrophysical parameters. Binary orbits in the nominal target systems are poorly characterized, including several cases where Gaia failed to confirm companions reported in double star catalogs. Limited far-UV and X-ray observations of IROUV targets.

#3 Understanding the Abundance and Distribution of Exozodiacal Dust

Gap Summary: Exozodi is interplanetary dust in circumstellar habitable zones, created by small-body collisions and cometary outgassing. Reflected light from exozodi can be much brighter than exoplanetary signals that IROUV is being designed to measure.

Relevance to Mission Architecture: Exozodi is a noise source that significantly affects exposure times for spectral characterization of small rocky exoplanets, and which can preclude exoplanet detections in some systems. Structure in the spatial distribution of exozodi can mimic the presence of a small exoplanet. While mission yields are only weakly dependent on exozodi levels, other possible metrics show stronger effects.

Capability Needed: Statistical knowledge of exozodi brightness levels among FGK stars, and for specific IROUV mission targets, with significantly reduced uncertainties over LBTI results. Theoretical understanding of exozodi sources, sinks, dust transport processes, and dynamical sculpting by planets. The ability to filter and remove exozodi from images to produce clean exoplanet spectra.

Capability Today: Detailed images exist for a large number of debris disks (cold exo-Kuiper Belts), but hardly any for warm dust near the habitable zone. The LBTI result of a median exozodi level 3x the solar system (Ertel et al. 2020 AJ 159 177) has large uncertainties and there is relatively poor sensitivity on individual targets. It is currently unclear whether the presence of hot dust in some systems poses a threat or not to detection of temperate rocky exoplanets.

#4 Planetary System Architectures

Gap Summary: The structure of planetary systems (number of planets, their masses, radii, and orbital elements), as measured by various techniques for different host star types and environments, is important for setting the context for conditions in the habitable zone and more generally, for defining the range of outcomes of planet formation processes.

Relevance to Mission Architecture: The observed demographics of planetary system architectures need to be understood in order to predict the science yields for exoplanet direct imaging as a function of IROUV starlight suppression requirements.

Capability Needed: Integrated exoplanet demographic results from radial velocity, transit, direct imaging, and microlensing surveys that can constrain and thereby improve population synthesis models for planetary system formation and evolution.

Capability Today: Ongoing TESS mission survey and its followup/validation of exoplanet candidates. Community efforts to follow-up accelerating stars identified between the Gaia & Hipparcos datasets. Radial velocity surveys. ALMA studies of the structure of protoplanetary disks, and high contrast imaging searches for self-luminous exoplanets.

#5 Eta-Earth: Occurrence Rate of Rocky Planets in Habitable Zone

<u>Gap Summary:</u> The occurrence rate of rocky exoplanets in the habitable zones of FGK stars ($\eta_\oplus$ or "eta-Earth") is a crucial parameter that defines the needed scope for the IROUV exoplanet survey. $\eta_\oplus$ remains considerably uncertain, with values ranging over nearly an order of magnitude. Better determinations will reduce uncertainty in estimated science yields (detection, spectroscopy) and would reduce the risk that IROUV might not achieve ~25 spectrally characterized potentially habitable exoplanets called for by Astro2020.

<u>Relevance to Mission Architecture:</u> Astro2020 envisioned IROUV to have an aperture of at least 6m, with the expectation that it could survey "*approximately 100 nearby stars, and successfully detect potentially habitable planets around at least a quarter of the systems*." The yield of rocky exoplanet planets in the habitable zone (defined in Decadal Fig. 7.6 to be 0.8-1.4 Earth radii planets between 0.95-1.67 au, understood to be for a solar twin and scaled by square root of stellar luminosity for other stars) scales essentially linearly with $\eta_\oplus$.

<u>Capability Needed:</u>
Observations, archival data analysis, and supporting theoretical research supporting improvement in constraints on $\eta_\oplus$, reducing uncertainty and potential biases. Detections of temperate rocky planets, and observations which can confirm the existence of candidate temperate rocky planets in Kepler data upon which $\eta_\oplus$ critically relies. Analysis of occurrence rates taking into account final Kepler products and improved stellar parameters, such that remaining uncertainties are dominated by intrinsic Kepler systematics. Ideally the values would be constrained and cross-checked via datasets other than Kepler, and trends sought as a function of system properties (e.g., stellar mass, multiplicity, presence of larger planets, etc.) to improve the fidelity of yield estimates.

<u>Capability Today:</u> Astro2020 adopted $\eta_\oplus = 0.24$. Multiple published estimates of $\eta_\oplus$ based on the Kepler data range widely over approximately one order of magnitude.

#6 Performance Simulations for the IROUV Exoplanet Survey

Gap Summary: A survey for temperate rocky exoplanets in more than 100 nearby habitable zones will be the largest single observing program of the IROUV mission. An accurate definition of this survey will allow Astro2020's goal of characterizing ~25 temperate rocky exoplanets to be achieved while preserving IROUV mission time for other priority science programs.

Relevance to Mission Architecture: Accurate simulations of this survey's detection performance, duration, observation cadence, and the utility of supporting information will be crucial for evaluating mission architecture options and operations scenarios.

Capability Needed: Definition and community agreement on the metric(s) that will be used to quantify the survey performance. Open-source code for the simulator with provision for community contributions. Consensus on the input values of key astrophysical and instrument performance parameters. Quantification of uncertainties in the results.

Capability Today: Adaptive Yield Optimization code employed in the HabEx and LUVOIR large mission studies by Stark et al. 2019 JATIS 5 4009.
Public ExoSIMs code developed under the WFIRST Preparatory Science program by Savranksy & Garrett 2016 JATIS 2 1006, and applied in an independent analysis of LUVOIR and Habex yields by Morgan et al. 2019 11117 01.

#7 Exoplanet Spectral Signature Extraction

Gap Summary: Systematic instrumental effects in IROUV high contrast images will limit the ability to extract reliable exoplanet spectra amidst backgrounds of exozodi or residual stellar speckles. The measured values of empirical parameters such as spectral slopes and linewidths can be affected, and the achieved spectral sensitivity may be worse than the photon noise limit.

Relevance to Mission Architecture: The post-processing sensitivity of exoplanet spectral measurements will depend on the achieved system stability and the calibration approaches that are used. These must be understood in order for IROUV to fulfill its measurement requirements.

Capability Needed: Ability to reliably extract physical parameters, such as the atmospheric pressure-temperature profile and abundances of major atmospheric constituents. Thorough understanding of the limits of the data, including effects of correlated and systematic noise sources. Strategies for data taking, calibration, and processing to mitigate these issues for IROUV, based on lessons learned from prior work.

Capability Today: Community analyses of coronagraphic imaging data from HST, JWST, and ground adaptive optics (e.g., GPI & SPHERE). Simple noise models predict coronagraphic spectra. Established practices for acquiring exoplanet spectra, post-processing of the data, and understanding how stellar speckles limit the extraction of space-based imaging spectra of exoplanets (e.g., Rizzo et al. 2018, SPIE, 10698). ExoPAG SAG 19 report defined new approaches to detection significance in high contrast imaging datasets.

#8 Properties of atoms, molecules, and aerosols in exoplanet atmospheres

Gap Summary: Exoplanet atmosphere models rely on an understanding of the optical properties of atoms, molecules and aerosols, as well as the reaction rates between relevant chemical species.

Relevance to Mission Architecture: The use of reflected light spectra to understand the composition and climate of exoplanets is a major goal of the IROUV mission, and depends on accurate input data to atmosphere models. Uncertainties in these data can affect the spectral resolution and S/N requirements for the mission measurements.

Capability Needed: Ability to perform theoretical calculations of key molecular and atomic spectroscopic properties, and/or laboratory measurements of gas spectra, reactions rate coefficients, and aerosol properties in relevant physical conditions. See white paper by Fortney et al. (2016; arXiv: 1602.06305)

Capability Today: Ab initio line list calculations of several dozen molecules with the ability to correct line positions. Laboratory measurements of line lists at low temperatures. Reaction rate coefficients measured at high combustion temperatures and standard Earth temperatures. Publicly available databases on molecular opacities and aerosol refractive indices (e.g. HITRAN).

#9 Simulations to relate science goals to architecture properties

Gap Summary: Tools are needed to simulate the performance of decadal survey science goals, and their response to top-level architecture properties such as wavelength range and aperture size.

Relevance to Mission Architecture: This is critical for architecture/cost/risk assessments. Crucial for mapping decadal science priorities to the architectures, and understanding how changes in architecture impact delivery of decadal science goals.

Capability Needed: Simulation tools for any of the IROUV (or other FGO) capabilities to deliver decadal science goals. These tools will be essential for understanding the trades the future project offices will be confronted with.

Capability Today: There are existing tools to understand the *detection* phase of exoplanet direct imaging. But we do not have tools for most of the other science cases, nor do we have them for exoplanet characterization.

#10 Probe the origin of the elements by determining the properties and end states of the first generations of stars and supernovae.

<u>Gap Summary:</u> Need to identify a set of several hundred candidate target stars at AB ≥ 14 mag in Galactic halo to enable measurements of the variation in r-process element creation and Galactic enrichment both spatially and across cosmic time, thereby determining the properties and end states of the first generations of stars and supernovae.

<u>Relevance to Mission Architecture:</u> Definition of what targets are available will define wavelength coverage, required spectral resolution, and necessary throughput to achieve desired SNR – and will affect observing efficiency and choices of optical design/aperture/coatings.

<u>Capability Needed:</u> The most metal-poor r-process-enhanced stars provide an effective avenue for investigation of open questions about the frequency, detailed physics, and yields of the primary astrophysical events associated with r-process nucleosynthesis as each one reflects the yield of an individual r-process event that occurred in the early universe.

<u>Capability Today:</u> Such metal-poor stars preferentially reside in the Galactic halo and comprise ~3–5% of all metal-poor halo stars in the Milky Way. As members of the Galactic halo population, all but a few r-process-enhanced stars are too distant for practical UV spectroscopy with HST. The practical magnitude limit for collecting high-resolution UV spectra with STIS is AB ~10 mag.

#11 Extragalactic source confusion in the far-infrared

Gap Summary: What is the effect of source confusion on the possibility of extracting desired scientific information from the extragalactic sky? For a diffraction-limited single-aperture telescope, the answer depends on both the distribution of FIR sources on the sky and the mirror diameter. Modeling and predictions have potential to inform the choices we'll make when designing a future far-IR space telescope.

Relevance to Mission Architecture: The telescope aperture size affects the possibility of extracting useful information to answer key science questions. Preliminary blind tests conducted for the Origins Large Mission Study suggest there are threshold aperture sizes below which a given science goal (e.g., extragalactic surveys; exoplanet biosignatures) cannot be accomplished. The Decadal Survey suggested that the Far-IR Great Observatory should be descoped relative to the proposed Origins Space Telescope. How small can the telescope be before the science case is compromised? Cost depends strongly on telescope size.

Capability Needed: A detailed study of the efficacy of spectral source "de-confusion" and science extraction for key science themes prioritized by the Decadal Survey, utilizing new FIR sky models anchored to best available data (JWST, Roman, IRAS, Herschel,..) and done as a function of telescope primary diameter.

Capability Today: A good sky model exists (coded in IDL), but the fidelity could be further improved (e.g., tie to new JWST observations). Preliminary blind tests were conducted for the Origins Large Mission Study.

#12 Understanding H2O, HD, atomic C/N/O in Protoplanetary disks

Gap Summary: The total mass of planet-forming disks is largely unconstrained and sets the timescale for planet formation – how long is enough material present to form planets? The abundance of water and other volatiles in disks is unknown and sets the initial compositional conditions for planet formation. To inform future missions that will answer these questions, a better understanding of the predicted exciting temperature, line strengths, line widths, and spectral signatures of various chemical species in protoplanetary systems is needed.

Relevance to Mission Architecture: Will inform trades on sensitivity (i.e., aperture size) and spectral resolution (i.e., required spectral resolution to obtain accurate measurements of masses, temperature, etc.) in the ~30-300um band needed to perform gross line intensity and tomographic mapping.

Capability Needed: Modeling of degeneracies between emission radial location (traceable to spectral resolution) and determined disk mass. Modeling of which water lines are expected to be detected in different environments (ISM, disks, comets). Balloon missions (e.g., ASTHROS) could observe 112 μm HD line in the brightest sources (e.g., TW Hydra).

Capability Today: Measurements of a limited number of systems by Herschel. Modeling via thermal-chemical codes such as DALI.

#13 Lab Astro Measurements of Dust and Ice

Gap Summary: We do not understand the spectral properties of dust and ice as a function of their formation, environment, morphology, and contaminants (CO, CO2, etc.) well enough to predict what features we expect to observe.

Relevance to Mission Architecture: Will inform choice of wavelength range, sensitivity (depending on line strength) and spectral resolving power.

Capability Needed: Laboratory measurements of dust grain and ice sludge morphology and spectra, modeling in different environments (ISM, protoplanetary disks), and balloon measurements of limited samples of targets.

Capability Today: NIR and MIR spectroscopy of dust grains and ice sludges.

#14 Modeling Feedback in Galaxy Evolution to better understand impact of magnetic fields and outflows

Gap Summary: Feedback plays a critical role in galaxy evolution but it is not well understood. Feedback is understood to be a critical component of galactic evolution, especially the impact of magnetic fields and outflows. However, the details of how these processes modify or govern evolution are not well understood. In particular, outflows are multi-phase, with a large number of potential critical probes in the far-IR, including rest-frame fine-structure lines, molecular absorption features and redshifted warm molecular gas lines.

Relevance to Mission Architecture: Motivates the addition of polarimetric capabilities (magnetic fields), and will inform choice of wavelength coverage and spectral resolution (outflows).

Capability Needed: Improved hydrodynamical models of feedback and outflows, including of the cool/warm phase, and coupling of these models to JWST and ALMA observations of the brightest targets and polarimetric observations at 1 - 300 µm.

Capability Today: Hydrodynamic models of feedback are continuously evolving and getting more detailed, but they generally lack testable predictions of key MIR/FIR lines.

#15 Understanding dust and gas in galaxies

Gap Summary: We do not have a good understanding of the physical properties of dust and gas in galaxies, especially at high redshift, and how this influences star formation and galaxy evolution. For example, predicting source counts for a blind survey is complicated by the limited understanding of far-IR line luminosity functions at $z>0$-3. This can be mitigated by further characterizing far-IR line properties around cosmic noon, and constraining semi-analytic models (SAMs) or hydro simulations with realistic prescriptions for far-IR source properties.

Relevance to Mission Architecture: Would set lower bounds of spectral resolution given expected line widths, determine spectral observing modes most likely to yield detections in a blind survey, and inform choice of field of view.

Capability Needed: Targeted ALMA surveys of small samples, realistic dust and gas modeling in simulations. Mid- and Far-IR (20-100µm) low-resolution (R~ "a few hundreds" to "a few thousands") spectroscopic mapping capability with sufficient sensitivity to detect unidentified infrared (UIR) emission features in galaxies at z~6.

Capability Today: ALMA targeted follow up of individual galaxies in Bands 9 and 10. JWST enables spectroscopy of UIR bands up to z~2 (limited by wave coverage up to 28µm). Realistic gas and dust modeling in SAMs/simulations.

#16 Black holes at the cosmic dawn: expectations for the early SMBH populations

Gap Summary: Detection of high-redshift SMBH are limited to the most luminous sources detected in optical surveys. There is the need to better understand how to use X-ray and corresponding multiwavelength observations to detect and characterize accreting high-redshift ($z>8$-10) supermassive black holes to then calibrate the predictions of black hole formation models.

Relevance to Mission Architecture: Detection of high-z black holes is the primary driver for the sensitivity requirement, angular resolution (required to associate the multiwavelength counterpart), mirror effective area, and field of view (large area is needed to detect rare sources). The angular resolution and effective area are primary cost and technical risk drivers.

Capability Needed: High-fidelity models and simulations for formation of first black holes and their growth to predict numbers, luminosity, and masses at $z >\sim 10$, as well as for $z\sim 6$-7. Develop modeling of subsequent SMBH evolution to compare and match with current detections at $z\sim 6$ and $z\sim 7$. Develop understanding of the multiwavelength emission from early SMBH to calibrate a relation between the observed X-ray flux and the object mass.

Capability Today: A set of theoretical models of SMBH seed formation and early evolution, with simplistic treatment of their accretion and emission properties. Chandra and XMM-Newton observations of $z=6$-7 sources limited to the brightest AGN/quasars detected in optical and NIR spectroscopic surveys.

#17 SMBH spin and mass measurements across a wide range of mass, luminosity, and redshift

Gap Summary: SMBH spin and mass are mainly known only for few bright and luminous sources. Measuring the BH spin for sources spanning a broad range of masses, luminosities, and redshift will allow a better understanding of BH accretion and physics.

Relevance to Mission Architecture: Depends on effective area requirements (many tens of thousands of photons are needed to achieve an high S/N ratio to separate the line from the continuum) and spectral resolution (to isolate the broad line by resolving the narrow components around it in emission and absorption, to have good resolution on the broad feature itself to correctly model its morphology, which depends non-trivially on several different factors e.g., disk emissivity, radial extent and inclination angle, iron abundance, black hole spin, coronal height). Spatial resolution would be important for localizing and following up GW detections from merging systems.

Capability Needed: Better understanding of how the accretion flow operates in different Eddington regimes, for example. What will be the observational signatures of different types of disk (thin vs. slim or thick), and what instrumental capabilities are needed in order to differentiate between reflection features produced from these states. Another is the exact nature of the corona (geometrically and energetically), and how its properties influence the irradiation of the inner disk and thus the reflection spectrum. More theoretical work is needed in understanding the nature of the corona (geometrically and energetically), and how its properties influence the irradiation of the inner disk and thus the reflection spectrum. Joint XRISM and XMM/Chandra and NuSTAR observations to show off the capabilities of a calorimeter. To foster synergies with GW detections, better simulations and modeling of merging SMBH binaries and their EM signatures is also needed as well as making the models public.

Capability Today: Current predictions are mainly based on thin disk models and some slim disk models, which are slowly incorporating some variations of e.g., density and ionization but not at the level needed to support strong predictions. Few (if any) EM models of merging SMBH systems are publicly available.

#18 Improved understanding of the relation between X-ray Binary emission, galaxy properties and theoretical predictions

Gap Summary: The X-ray binary population is a unique observational signature of galaxy properties (e.g., star formation and galaxy mass), and one of the key factors contributing to the cosmic reionization history at z=10-20. Exploiting their full potential requires work on questions such as: How to best relate the X-ray binary population to the host galaxy properties (such as star formation rate, host galaxy mass, age and metallicity of stellar population)? How to extrapolate the knowledge of the X-ray binary population at z=0-6 to the very high redshift Universe at z=8-20?

Relevance to Mission Architecture: Detection of X-ray emission from very high-redshift galaxies due to X-ray binaries strongly drive the sensitivity of the mission in the soft X-ray energy band. Moreover, high angular resolution would allow the to resolve the direct emission from X-ray binaries in galaxies well beyond the local universe.

Capability Needed: The number of X-ray binaries per unit of stellar mass as the function of their age is one of the most sensitive tools that we have to constrain binary evolutionary models. Therefore deeper Chandra observations of galaxies to resolve their X-ray binary population is important to fine tune model parameters (such as kick velocity distributions, common envelope efficiency, stellar wind strengths) and thus to improve those evolutionary models and their predictions for high-redshift galaxies.
Robust understanding of the integrated X-ray binary emission in high-redshift galaxies, as a function of galaxy properties is needed in particular separating the binary from the central super massive black hole emission. By better constraining the hard X-ray spectrum (using e.g., NuSTAR) of nearby X-ray binaries, we will be better equipped to understand the observed spectrum in the soft X-rays for both X-ray binaries identified at higher redshift and also the soft X-ray integrated spectrum of high redshift galaxies.
Reliable and well-constrained models are required, which can be achieved only by fine tuning their parameters with such observations.

Capability Today: Strong detections of X-ray binaries with Chandra and XMM-Newton in local galaxies as well as results from stacking analysis of higher redshift galaxies, extending to z=~3. Spatially resolved measurements in the closest galaxies. Theoretical models are available and can reproduce observations in the local Universe but when compared with observations for high redshift galaxies it remains unclear if an evolution of the X-ray binary formation with redshift is observed or not.
