The following gap list represents a synthesis of inputs gathered from precursor science workshops, "Precursors to Pathways: Science Enabling NASA Astrophysics Future Great Observatories" held in April and October 2022, as well as community feedback received throughout the second semester of 2023. The workshops aimed to facilitate discussions that would shape a comprehensive list of needed investigations, crucial for defining the performance and architectures of future observatories. In the summer of 2023, the Astrophysics Programs (Exoplanet Exploration, Physics of the Cosmos, and Cosmic Origins) issued a call for additional community inputs to further enrich the precursor science gap list for Future Great Observatories.

The updated list presented here incorporates both the gaps shared with the community prior to the previous ROSES deadline as well as the newly identified gaps.

The scientific areas with the potential to significantly impact mission architecture included in the gaps can be summarized as follows:

- Modeling of target spectra, and the 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 to achieve the mission's main science goals, 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, 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.

- Development of theoretical models and simulations that improves the knowledge of number counts, spectral shapes and emission of astrophysical sources of interest, to better constrain the mission architecture.

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#1 Modeling Exoplanet Atmospheres and Biosignatures

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

Relevance to Mission Architecture: Modeling informs the spectral resolution, wavelength coverage, and signal to noise ratios needed for HWO 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.

Capability Needed: 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.

Capability Today: 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 HWO Exoplanet Imaging Targets

Gap Summary: Improve knowledge of plausible HWO 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 HWO target stars can improve the fidelity of exoplanet yields estimates used for architecture trades. If a significant fraction of nominal HWO 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 likely HWO 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. A uniform compilation of fundamental stellar properties such as Teff, radius, and chemical abundances. 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 HWO 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 HWO targets, and inhomogeneous datasets of fundamental stellar properties.

#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 HWO 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 HWO 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 Mitigating Stellar Jitter as a Limitation to Exoplanet Dynamical Measurements

Gap Summary: Measurements of masses and orbits are crucial for characterizing exoplanets, and for modeling their spectra and composition (interpreting biosignatures). Precision radial velocity (PRV) and astrometry are anticipated to be the primary means of measuring masses in support of HWO reconnaissance of exoplanet atmospheres. Both techniques suffer from stellar noise ("jitter") from multiple sources over a range of timescales, and for PRV the stellar noise currently dominates the uncertainty budget below 1 m/s - currently precluding reliable detection of temperate Earth-mass exoplanets around Sun-like stars.

PRV could provide a mix of preparatory and/or follow-up capability for detecting planets (including small potentially habitable worlds), constraining their orbits and measuring masses. The degree to which EPRV can contribute capability for characterizing ~Earth-mass temperate planets by the time of HWO is unclear (although the ExEP EPRV Working Group has presented a community pathway). This is a precursor science topic as advancing EPRV and astrometry techniques, or improving our knowledge of their limitations for implementation, can inform the strategy for designing the HWO observatory or complementary capabilities needed to provide preparatory of followup mass/orbit measurements.

Relevance to Mission Architecture: Advancing the Extreme Precision Radial Velocity (EPRV) method to enable reliable detection of velocity amplitudes of ~<10 cm/s could potentially detect and measure masses of Earth analogs orbiting Sun-like HWO targets. Prior knowledge of planet orbits and ephemerides would allow the HWO exoplanet survey to proceed more quickly, enabling the highest impact science earlier in the HWO mission. If technology goal sub-microarcsecond-level astrometry is achievable, and astrometric jitter could be mitigated, then astrometry could provide an alternative method which could yield orbits and masses for rocky planets around nearby stars. The LUVOIR concept study baselined microarcsecond relative astrometry capability. The progress (or lack thereof) towards measuring <10 cm/s radial velocity amplitudes will factor into a decision on how aggressively astrometry needs to be developed to support mass determinations for HWO targets.

Capability Needed: Agreement on the supporting "mass determination strategy" for the HWO exoplanet survey - exactly what precision is needed to interpret reflected light spectra of potentially habitable worlds, and how might it best be obtained? Further advancement in the precision of both the RV and astrometry techniques. to inform choices for supporting projects for preparatory surveys to support HWO spectroscopic reconnaissance of the nearest potentially habitable worlds. The Extreme Precision Radial Velocity Working Group Final Report (2021) provided a roadmap to NASA and NSF for advancing the EPRV technique in support of a direct imaging space telescope (i.e., HWO). Among the nearest, brightest plausible ~100 HWO targets for a survey of potentially habitable worlds, the median target is a 5th magnitude Sun-like (G2V, 1.0

Msun) star at d=10 pc, and an Earth twin would produce a radial velocity amplitude of ~9 cm/s (independent of distance & brightness) or astrometric amplitude of 0.3 microarcsec.

Capability Today: Single measurement precision among state-of-the-art PRV spectrographs is approaching ~30 cm/s (e.g. ESPRESSO, EXPRES, NEID), however radial velocity noise varies from star to star due to activity, rotation, temperature, and survey gravity: a typical RMS values is ~1 m/s. The smallest claimed RV amplitudes detected today are ~35 cm/s for Tau Ceti (Feng *et al.* 2017, AJ, 154, 135). Collier Cameron *et al.* (2021, MNRAS, 505, 1699) demonstrated the feasibility of reliably measuring RV signals with amplitudes of 40 cm/s for the Sun. Gaia should enable detection of large planets on long periods with amplitudes of typically >100 microarcseconds (Perryman *et al*. 2014, ApJ, 797, 14), but very few among bright stars (like HWO targets).

#5 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 HWO 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.

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

Gap Summary: 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 HWO 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 HWO might not achieve ~25 spectrally characterized potentially habitable exoplanets called for by Astro2020.

Relevance to Mission Architecture: Astro2020 envisioned HWO 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 $\eta_\oplus$.

Capability Needed: 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.

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

#7 Performance Simulations for the HWO 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 HWO mission. An accurate definition of this survey will allow Astro2020's goal of characterizing ~25 temperate rocky exoplanets to be achieved while preserving HWO 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.

#8 Exoplanet Spectral Signature Extraction

Gap Summary: Systematic instrumental effects in HWO 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 for HWO 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 HWO, 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.

#9 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 HWO 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).

#10 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.

#11 Low Surface Brightness Disk Galaxies in the Local Universe

Gap Summary: Where are the large low surface brightness (LSB) disk galaxies in the local volume (D<100 Mpc) and what are they like? These ghostly galaxies are difficult to detect and characterize. The first step in understanding their properties is to find them in the extraordinary imaging datasets now or soon to be available. Equally important is to quantify the selection function: what galaxies are detectable? We know of some of these galaxies, but their selection function depends on field crowding as well as position on the sky. Their volume density is therefore difficult to constrain. All present samples are incomplete and fragmented. Closing this gap requires creating a robust catalog of LSB galaxies and knowing their luminosities, sizes, and surface brightness parameters.

Relevance to Mission Architecture: The science gap informs the instrument design and makes a case for Multi-Object Spectroscopy over a large field of view. There are precedents for FOV of the multiobject UV spectrograph for HWO: HabEx chose "> 2.5 x2.5 arcmin" (page 5-19 of their final report) and LUVOIR chose "2x2 arcmin" (page 8-42 of their final report). Due to lack of knowledge of the number and size of targets, the trade-off between program duration and optimal patrol field remains unknown. This would inform the FOV required for MOS spectroscopy, and spatial and spectral resolutions for the spectrograph to be able to use it to characterize the stellar populations and kinematics of the LSBs.

Capability Needed: Collate existing data sets into a clear catalog with an unambiguous selection function.

Capability Today: There is not a clear catalog. Some (older) work has been done, or specifically for a given survey (e.g. edge-on in DES) but a more uniform catalog of low surface brightness disks does not exist.

#12 Mapping UV Emission in Nearby Star-Forming Galaxies

Gap Summary: Deciphering the synergy between stars and gas is fundamental in providing a deep understanding of galaxy evolution. It is essential to map the high ionization UV emission in nearby star-forming galaxies in order to understand the feedback processes that link massive stars with their surrounding ISM. To prepare for such observations with HWO, there is a need for high resolution, galaxy scale hydrodynamical simulations that resolves massive stars and the effects of their high-energy photoionizing emission on the surrounding gas. Simulating IFU observations of these structures, in the UV wavelengths, will yield theoretical expectations on the extent of UV emission features from both the gas and stars. This can only be achieved in the UV where these signatures lie, on spatial scales that allow us to isolate faint UV emission, with spectral resolution that allows us to map outflow kinematics.

Relevance to Mission Architecture: Closing this gap advocates for a UV-IFU, a unique capability that does not exist. The study will inform the field of view, spatial and spectral resolution, and wavelength coverage required for a UV-IFU on HWO. Simulated UV spectra will help us explore the extent to which spatial variations in UV properties can be traced, thus informing us on the tradeoff between IFU vs MOS designs, and subsequently the scientific questions answerable within the limitation of each design.

Capability Needed: High resolution, galaxy scale hydrodynamical simulations of individual galaxies to (i) recreate galaxies with spatial variations in chemical/physical properties that match those seen in optical IFU observations and (ii) provide synthetic UV spectra spatially across the same systems. These will be used to provide simulations of the UV-IFU observations, with rest-UV spectra across each system. Ground-based optical IFU observations (archival) can provide a basis for the models.

Capability Today: There is no suitable data currently. Simulated galaxies exist (eg. in FOGGIE simulations), but there is a need to post-process the outputs to create simulated UV and optical spectra of the galaxies.

#13 Modeling the interaction of multiphase galactic winds with a realistic CGM

Gap Summary: Feedback associated with star formation is central to the regulation of galaxy evolution, but there is significant tension in our current models for how this feedback works in practice—particularly in regard to the driving of galactic winds. Cosmological simulations and SAMs all require ejective feedback with mass fluxes exceeding the SFR, whereas observations and high-resolution small-scale simulations favor a preventative feedback in which the outflows carry much less mass but large amounts of energy. In order to reconcile these pictures we need models for how multiphase winds shaped by complex microphysics interact with a realistic CGM. These models will allow us to make accurate mock observations that can be used to inform the wavelength coverage and spectral resolution.

Relevance to Mission Architecture: Predictive models are needed to determine what wavelength ranges and spectral resolutions are necessary to make the most constraining observations.

Capability Needed: Improved magnetohydrodynamic models of galactic winds interacting with the CGM, which include realistic microphysics (e.g. magnetic fields, cosmic rays and radiative transfer) and are accurately forward modeled into the observational space. Spatial resolution needs to be ~ 1 pc to capture the essential physics of mixing and cooling that regulate the phase structure and control the observables.

Capability Today: Existing models fall into two categories: Idealized isolated galaxies or patches of galaxies that launch outflows into a vacuum, and cosmological simulations. The former has the advantage of high resolution and the ability to include more physical processes but cannot be used to make observational predictions of the wind-CGM interaction since there is no CGM. While the latter has the advantage of the global context which is essential for capturing the wind CGM interaction, but due to the extreme computational expense can only be run with limited physical processes and limited resolution. The current state of the art for global simulations in terms of spatial resolution is about 100 - 1,000 pc in the inner CGM / disk-halo interface.

#14 Improving our understanding of young massive stellar populations in metal-poor environments

Gap Summary: We do not have yet a good understanding of stellar populations in low-metallicity (Z<0.5Z_sun) environments, particularly their young and (very) massive members. We continuously find that our theoretical populations synthesis models widely employed to interpret far-UV spectroscopy of unresolved young massive stellar populations in star-forming galaxies are unable to successfully reproduce the features in their observations. Theoretical population synthesis models are improving constantly, although still struggling to reproduce the low-metallicity stellar population spectra, however, there is an obvious lack of empirical observations of individual metal-poor stars to guide the physics adopted in the models. This is due to our lack of knowledge on the treatment of mass-loss in very massive stars at low metallicities and the lack of metal-poor templates. This specific science gap greatly limits our understanding of galaxy evolution and interpretation of stellar population observations not only in the local universe but at high redshift.

Relevance to Mission Architecture: This precursor science will inform the UVOIR choice of wavelength coverage (bluest range required for this science) and the minimum spectral resolution as both of these parameters are critical for improving our stellar population models in the low-metallicity regime. Studies in this area will also help inform the sensitivity requirements, particularly crucial in the FUV regime.

Capability Needed: A robust set of FUV-Optical spectroscopic observations of massive stars at low metallicities. We are currently limited by the sensitivity in the FUV of HST, which prevents us from collecting spectra of these objects beyond the LMC/SMC. The capability needed consists of access to a library of spectroscopic observations of massive stars (of different metallicities, specifically below SMC metallicity) with FUV-optical wavelength coverage, and medium resolution (R~20,000).

Capability Today: Theoretical population synthesis models are improving constantly, although still struggling to reproduce the low-metallicity stellar population spectra; however, there is an obvious lack of empirical observations of individual metal-poor stars to guide the physics adopted in the models. The capability at hand today is FUV spectra with HST at the needed spectral resolution and wavelength coverage: a limited number of FUV-optical spectra of massive stars. The few existing observations, external to the ULLYSES program, are also limited in the metallicity space probed.

#15 UV spectroscopy of nearby high-z analogues to understand the first galaxies

Gap Summary: Rest-frame UV spectra play a key role in the understanding of massive stellar populations, chemical evolution, feedback processes, and reionization. In particular, in the current JWST era, the UV spectroscopic frontier has been pushed to higher redshifts than ever before, to finally reveal the first galaxies in the distant Universe. It is thus fundamental to understand the diagnostic power of UV lines (e.g., Lya, CIV ll1548,1551, HeII l1640, OIII] ll1661,66 and CIII] ll1907,09). UV spectra of local high-z analogues represent a powerful ideal laboratory, thanks to the level of data quality and spatial resolution the local Universe can offer. Tracing their spatial distribution would allow us to isolate the sources of the UV photons within these systems.

Relevance to Mission Architecture: UV integral field spectroscopy (IFS) represents the future of UV spectroscopy. At optical wavelengths, the advent of IFS allowed to build spatially resolved diagnostics to investigate the gas properties, including the main ionization sources. Most importantly, optical IFS allowed to carry out detailed chemo-dynamic studies, to connect the kinematics of the gas in galaxies to the spatial distribution of the metal content, thus studying the effect of stellar and active galactic nuclei feedback in galaxies. Analogously, large-scale UV IFS would allow us to perform similar chemo-dynamic studies with UV diagnostics of nearby high-z analogues at pc-scales for the first time. This is crucial to interpret high-z spatially resolved spectra in the rest-frame UV revealed with IR and optical observatories (including JWST/NIRSpec-IFU, the future ELTs and the IR/optical side of the IROUV future NASA facility). In order to design a UV IFU for a future mission we need to know the needed field of view, sensitivity, spectral and spatial resolution.

Capability Needed: The use of HST UV spectroscopy and imaging to inform the IFU design of a future UVOIR observatory represents the needed capabilities to close this science gap. On the one hand, the high sensitivity and spectral resolution of many archival HST/COS data provide us with high signal-to-noise UV spectra to investigate the presence and strengths of UV lines in high-z analogs. On the other, archival HST imaging data (with ACS SBC and STIS) can be used to map UV spectral features, to understand their morphology and extent.

Capability Today: Currently, several nearby galaxies considered high-z analogs have been observed with HST/COS (e.g., the CLASSY and LzLCS surveys). Also, some of them have been mapped in Lya, using HST/ACS SBC, revealing the presence of extended and faint UV haloes around these systems. Only recently ACS SBC has started to be used to map CIV, while STIS imaging capabilities are available but have rarely been explored. Overall, none of the current UV studies have used UV spectra and UV emission line maps to define the sensitivity, spatial and spectral resolution, and field-of-view that a future UV IFU would need to trace these important UV emission lines.

#16 Tracing Intermediate Temperature Gas with High-Ionization Emission Lines

Gap Summary: The injection of turbulence into the interstellar medium (ISM) and the exchange of energy among its different phases is of critical importance for our understanding of galaxy evolution. Processes happen in fast supernova shocks and in mixing layers between hot (>10^6 K) and warm (~10^4 K) gas due to galactic outflows and inflows. The collisionally excited emission from "intermediate temperature" regions is best traced by the OVI 1032,1038 Å doublet, which is typically uncontaminated by photoionized gas. Other lines expected from these regions include corresponding doublets from SVI 933,944 Å, NV 1238,1242 Å, SiIV 1393,1402 Å, and CIV 1548,1550 Å, which may be used also to probe the elemental abundances. While the microphysics of the processes responsible for the emission are well established, and have been studied in specific and localized contexts such as in individual supernova remnants and superbubbles and a handful of high-velocity cloud boundaries, the available data is limited. Importantly we lack a framework for interpreting observations of these lines on larger (kilo-parsec) scales where the dynamics becomes complex.

Relevance to Mission Architecture: Through detailed hydrodynamical modeling and incorporating accurate atomic physics of UV emission, model predictions will inform the spectral resolution that will be required to separate velocity components, and the spectroscopic modes that will ensure the optimal simultaneous coverage both in space and wavelength.

Capability Needed: A hydrodynamic code that will calculate line emission with sufficient spatial and velocity resolution to allow the use of FUV lines as diagnostics for the energy transfer, turbulence and metallicities. Wavelength coverage should go down at least to about 1000 Å so the O VI doublet is included, and ideally down to the Lyman limit at 912Å so the SVI lines may be studied.

Capability Today: There are a number of sophisticated hydrodynamic codes that can trace densities and temperatures on large scale at sufficient resolution, but they do not yet incorporate the atomic physics in sufficient detail to predict the OVI and other line emissivities. There is a limited amount of data in hand, mainly from the Far-Ultraviolet Spectroscopic Explorer (FUSE) for OVI and SVI, and from HST for NV and CIV, which can be used to inform models.

#17 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.

#18 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.

#19 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.

#20 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.

#21 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 >~10, as well as for z~6-7. Develop modeling of subsequent SMBH evolution to compare and match with current detections at z~6 and z~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.

#22 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 band. Moreover, high angular resolution would enable resolving of 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.

#23 Probe the corona emission in Active Galactic Nuclei at hard X-ray energies

Gap Summary: The extragalactic Cosmic X-ray Background (CXB) is predominantly attributed to Active Galactic Nuclei (AGN). Their X-ray emission is thought to be produced by hot electrons in the proximity of the central supermassive black hole (SMBH) in AGN, namely the corona. So far, hundreds of thousands of AGN have been detected in X-rays, yet, the properties of the X-ray corona are still unclear. The corona is measured to be a few gravitational radii close to the SMBH, therefore establishing a connection between the corona and the accretion of SMBH offers a unique opportunity to assess the extreme environment within a few gravitational radii of the SMBH. The most prominent feature of the corona in X-ray, the so-called high-energy cutoff (typically at 50-500 keV depending on luminosity), is mainly constrained by combining current soft and hard X-ray telescopes band coverage. The energy range and effective area necessary for a future X-ray great observatory to study AGN coronae in detail will be informed by knowing the high-energy cutoff of a population of AGN.

Relevance to Mission Architecture: Detection of the X-ray corona for a large sample of AGN over a broad range of luminosities and redshifts strongly drive the sensitivity of the mission and the band coverage. Energy coverage: extending to 20 keV could measure a cutoff at 120 keV (rest) for an AGN at $z=5$. Large effective area at high energies would allow to detected faint sources.

Capability Needed: A large (many tens of sources) sample of AGN spanning a wide range of luminosities and redshifts, with well-characterized spectra over a broad energy range is needed to define the properties of the corona. A systematic study of the AGN corona needs a broadband X-ray telescope with large effective area and low background covering 0.5-50 keV. With such a telescope, it would be possible to provide a full understanding of the corona, the main AGN X-ray emitter.

Capability Today: Only a handful of sources have well-measured coronal properties obtained by combining soft X-ray telescopes like Chandra with the hard X-ray telescope NuSTAR. NuSTAR covers only up to 80 keV (with high background at 24-80 keV, so providing a low signal-to-noise ratio at >24 keV). This sample with known corona properties is biased towards luminous sources mainly at high redshift where the cut-off is redshifted to energies <24 keV.

#24 Theoretical modeling of High Redshift Gamma-ray Bursts

Gap Summary: High-redshift gamma-ray bursts (GRBs) are a relatively unknown class of object. These cataclysmic events have the potential to shed light on the early universe up to redshifts of ~9, which is the current highest redshift GRB ever observed. An X-ray future great observatory can shed light on these objects if it is able to detect them and characterize their spectral shape, allowing for greater understanding of these events and their relation to GRBs in the nearby universe and understanding their potential use as probes of the high redshift universe. Theoretical modeling of high-redshift GRBs to predict their timescales, energetics, and spectral energy distributions has not been developed. These properties all play a role in determining the energy range and sensitivity needed for an X-ray future GO to characterize these events.

Relevance to Mission Architecture: The physics associated with high-redshift GRBs may differ from low-redshift GRBs, including for example the jet Lorentz factors, jet structure, and radiation mechanisms, to name a few. These differences can affect where the spectrum peaks and therefore the energy range in which a future great observatory would need to operate to detect as many of these events as is possible. Requirements on the field of view, field of regard, sensitivity, and response time will be informed by an understanding of the range of viable models for the rate, luminosity, and time evolution of high-redshift GRBs.

Capability Needed: Develop a set of theoretical models for high-redshift GRBs to describe their jet structures (ie Lorentz factors, energy distributions, etc) and provide predictions for their timescales, energetics, and spectral energy distributions that include a description of their (likely) Population III progenitors.

Capability Today: Theoretical models exist for low-redshift GRBs that can be extrapolated to high-redshift GRBs, but if the progenitors of high-redshift GRBs are Population III stars, then they are very different from the NS mergers/core-collapse supernovae which produce low-redshift GRBs. As a result, there are large uncertainties in being able to make inferences about high-redshift GRBs from low-redshift GRBs. There has recently been progress with JWST on understanding Population III stars. There have been advances in modeling the radiation that is emitted from low-redshift GRB jets. Overall, there are no robust models of high-redshift GRBs that can address their potential physical properties.

#25 Blazars across cosmic time: evolution of jetted AGN and theoretical interpretation

Gap Summary: The number density and luminosity distribution of blazars across different redshifts are not fully understood. At low redshifts, observations can identify blazars with low and high luminosity as well as misaligned jetted AGN (i.e., radio galaxies). But at high redshifts, current X-ray telescopes can only detect the brightest blazars.This results in significant biases about the blazar number density and luminosity at high redshifts, thus whether and how jetted AGN evolve in cosmic time cannot be constrained. Theoretical interpretations of the number density and luminosity of jetted AGN are left behind, merely empirical relations by fitting the observed (and probably biased) distributions are available.

Relevance to Mission Architecture: High sensitivity and angular resolution of future X-ray telescopes are needed to identify more blazars at higher redshifts and associate to multi-wavelength counterparts.

Capability Needed: Detailed numerical simulations that can calibrate the blazar power and multi-wavelength luminosity can reduce the observational biases towards brighter sources and guide the observational capability requirements for future X-ray telescopes. These global numerical simulations need significant theoretical efforts and computational resources. Preliminary studies of magnetohydrodynamic and particle transport simulations can provide solid physical basis for particle acceleration in jets. Radiation transfer simulations can help to constrain the multi-wavelength emission.

Capability Today: Number density and luminosity distributions of blazars below redshift of ~3 are reasonably covered by X-ray telescopes, but at higher redshifts the bias can become significant. Theoretical interpretations are merely empirical fittings of the observed distributions.

#26 Multi-messenger observations of extreme supermassive black holes

Gap Summary: While large samples of Active Galactic Nuclei have been detected thanks to large X-ray extragalactic surveys, discovery of more rare objects that require either cadenced large area surveys and/or higher cadence monitoring of a large sample remains lacking. The discovery of extreme black holes, like Tidal Disruption Events, Supermassive black hole binaries, Stellar mass black holes in AGN disks, Quasi-Periodic Eruptions and Changing Look AGN requires capabilities that we currently don't have. As a consequence, theoretical modeling of the above has proven to be difficult as it relies only on a few examples of each sources. For instance, detecting sub kpc binaries is very hard beyond the low-z Universe, and even then it requires high spatial resolution and long integrations of multiple targets. Quasi Period Eruptions are an exciting, new, potentially multi-messenger event, but with only 6 QPEs candidates, their origin remains debated (i.e. whether due to an Extreme Mass Ratio Inspiral event, or whether due to disk instabilities). Larger volume X-ray surveys (i.e. with wide area and sufficient sensitivity) at high-cadence are required to catch quasi periodic flares in a larger number of sources, and thus test the growing number of theoretical models.

Relevance to Mission Architecture: High sensitivity, large field of view and easy repointing and fast slewing capabilities are needed to study extreme and rare black holes.

Capability Needed: Good X-ray sensitivity and flexible scheduling/slew for rapid X-ray follow-up and cadenced monitoring of known sources, and large area, wide field-of-view surveys at soft X-rays for the X-ray discovery of new events. From a theoretical perspective, General Relativistic magnetohydrodynamical simulations of luminous accretion flows including radiation will enable predictions for light curves and spectra of extreme SMBH events.

Capability Today: eROSITA has a wide field of view and soft X-ray response, which is key for discovering new transients, but its 6-month cadence is insufficient. NICER and Swift have flexible scheduling but are not sensitive enough to reach larger horizon distances of LIGO/LISA. The LVC regularly discovers stellar mass black hole mergers, but the error circles are too large to identify host galaxies. Recently there have been great advancements in radiation hydro simulations of black hole accretion, thanks to GPUs.

#27 Understanding SMBH growth across cosmic time using black hole spin

Gap Summary: Measuring black hole angular momenta derived from, e.g., X-ray reflection spectroscopy, for sources spanning a broad range of masses, luminosities, and redshift and comparing against expectations from hydrodynamical cosmological simulations will allow a better understanding of BH accretion and physics.

Relevance to Mission Architecture: Impacts both the effective area requirements (e.g., for reflection spectroscopy, many tens of thousands of photons are needed to achieve a 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, and 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) and also bandpass (for high redshift sources or non-Fe line diagnostics).

Capability Needed: Deeper observations of individual sources to decrease the uncertainty on individual spin measurements and to increase the overall sample size are needed. These data would reduce model systematics, breaking parameter degeneracies and enabling both further exploration of parameter space and enhanced treatment of physics / geometries / realistic accretion flows. Furthermore, the microphysics of gas (atomic parameters, high-density plasma effects, etc.) needs to be improved. In addition, in order to turn spin parameter into a SMBH growth diagnostic, major cosmological simulation suites (e.g. IllustrisTNG, SIMBA, EAGLE) need to include consistent spin parameter evolution post-processing.lude consistent spin parameter evolution post-processing.

Capability Today: Currently, 46 spin parameters (including lower limits) with X-ray reflection spectroscopy have been measured. Several suites of large (~100 cMpc)^3 cosmological simulations with a range of treatments for baryonic physics, and AGN feedback subgrid modeling in particular, are available. Among these, only one suite to date post-processed to trace spin parameter evolution across cosmic time in a large statistical sample of SMBH down to redshift z=0 (~6000 in Horizon-AGN). A working framework for reflection spectroscopy including relativistic effects for spin parameter recovery (e.g., XILLVER/RELXILL) has been developed.

#28 Improving the Understanding of Jet Launching Regions in Astrophysical Sources

Gap Summary: There is not a one-to-one connection between observations and theory regarding jets in general and specifically jet-launching regions. This is a time-intensive computational problem.

Relevance to Mission Architecture: Wavelength range, Spectroscopic modes/methods, Polarization, Imaging capability, Spatial Resolution.

Capability Needed: Capability needed is intensive 3-D computational modeling and simulations, with relativistic effects included. The models need to be self-consistent, including magnetic field effects and other relevant physics.

Capability Today: Currently available models include different physics, without being self-consistent. There is no modeling that has a complete physical picture of these relativistic jets.

#29 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 and X-ray, 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). Motivates the sensitivity in the soft X-ray band and large field-of-view.

Capability Needed: Improved hydrodynamical models of feedback and outflows, including of the cool/warm phase, and coupling of these models to JWST and ALMA and/or existing X-ray observatory 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.

#30 Atomic Data Needs for High-Resolution X-ray Spectroscopy

Gap Summary: X-ray spectroscopy is a powerful tool for studying extreme environments in astrophysical sources. The X-ray band simultaneously covers the emission and absorption of almost all astrophysically relevant elements, but its diagnostic potential relies strongly on the accuracy of the atomic data needed to produce reliable spectral models. The XRISM team has identified a long list of atomic data needs for the upcoming high spectral resolution observations. These needs will be exacerbated in the next decades when even larger missions fly micro-calorimeter detectors. This is a wide science gap that requires large and coordinated efforts on the experimental and computational sides of Laboratory X-ray Astrophysics.

Relevance to Mission Architecture: Developing better atomic databases will be a primary driver for spectroscopic resolution and energy range coverage.

Capability Needed: Calculations of large sets of inner-shell transitions for all astrophysically relevant ions (carbon through nickel) with accuracies that match the instrumental resolution of future micro-calorimeters are needed. Experimental measurements of similar atomic quantities are necessary to serve as a benchmark for calibrating both the atomic databases and the spectral models to be produced.

Capability Today: Several atomic databases and spectral models (both collisional and photoionization equilibrium) are publicly available (e.g., XSTAR, SPEX, AtomDB, Chianti, ADAS). Operational facilities are currently conducting laboratory measurements of atomic and plasma quantities at high energies and also developing integrated experiments that include plasma effects across a range of astrophysically relevant densities and temperatures (e.g., EBIT-I electron beam ion trap facility at Lawrence Livermore National Laboratory, and the OMEGA EP laser system, which is part of the OMEGA National Laser Users' Facility). Extensive spectral model grids are needed to support spectral fitting using artificial intelligence tools.