

## Cover Page

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Fundamental Materials Research

### Research Campaign: In-Situ, Resilient, and Sustainable Moon-to-Mars Construction

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**Background:** In 2020, NASA outlined the lunar surface sustainability core surface elements, including a lunar foundation surface habitat, to house four crewmembers [1]. NASA has been looking to advance 3D printing construction (3DPC) systems through the Moon-to-Mars Planetary Autonomous Construction Technology (MMPCAT) program [2]. The major research goal for MMPACT is to develop, deliver, and demonstrate on-demand capabilities to protect astronauts and create infrastructure on the lunar surface. In 2020, Marshall Space Flight Center (MSFC) published a conceptual design for a concrete lunar landing pad, utilizing 3DPC technologies [3] using lessons from the Apollo era and the Mars robotic missions. In 2021, the Kennedy Space Center (KSC) Granular Mechanics and Regolith Operations (GMRO) laboratory subsequently tested several granule-based materials for oxygen/methane rocket engine hot fringes [4]. KSC has identified eleven potential candidate materials, ranging from compacted regolith to sintered regolith by metal powder combustion. So far, only five of those materials have been tested.

This decadal campaign builds upon existing published data for Moon and Mars construction materials, testing, and in-space environmental experiments, and is proposing four major transdisciplinary themes to support NASA's 2023-2032 research missions related to the near-future Moon habitation. One major existing issue underlying all NASA's construction materials research is the cost of payloads and indigenous availability of materials. Any optimization for construction materials that would reduce the amount of payload necessary to build the infrastructure will drastically reduce the cost (current estimates: \$1.2M/Kg) [5]. Another major challenge that the proposed research addresses are the lunar environmental hazards such as moonquakes, micrometeoroid impact, dust, solar flares, microgravity, and thermal effects, which need to be considered besides the landing plumes. *Four major research themes need to be led to address these underlying and many other challenges: 1. Construction materials design and optimization based on availability, recyclability, durability, printability, and cost efficiency; 2. High-fidelity computational efforts to study the effects of extreme environmental conditions on materials' physical, chemical, and mechanical performance; 3. Validation of the environmental deterioration mechanisms on the physical, chemical, and mechanical properties of needed construction materials; 4. Performance optimization of on-ground, large-scale construction technologies to address biophysical sciences-related challenges, such as pore formation, reduced mobility, and reduced gravity, as well as validation of in-space, small-scale 3D printing processes. Generated data can be analyzed via artificial intelligence (AI) and utilized for purposes such as reconstruction of seismic wavefields related to moonquakes for future predictions, and data mining and data analytics for NASA's preliminary and ongoing studies. We propose a broad theme of future research activities that address several challenges based on NASA's ongoing and future research priorities.*

**Objectives:** (1) To identify, design, and optimize critical space infrastructure elements, utilizing mainly in-situ resources, to resist the extreme space environments; (2) To design, characterize, scale up, and optimize novel construction (concrete-like) materials to withstand the lunar surface environmental cycles; (3) To perform high-fidelity multiscale, multi-physics simulations for the assessment of the multi-hazard performance of optimized materials and infrastructure elements; (4) To perform multiscale, multifunctional characterization of infrastructure systems; (5) To validate the performance of the proposed designs utilizing existing and new Biological and Physical Sciences (BPS) platforms, on-ground and in-space for the performance of proposed related tasks; and (6) To develop AI models to provide predictive capabilities.

**Approach:** The sensitivity of the developed materials response will be established through a parametric evaluation of physical and environmental parameters to address space additive construction, including (1) Multiscale (atomic to macro) mechanics response via simulations and experiments; (2) Materials ultimate strength rate development for in-space environments, (3) Structural health monitoring during and post additive construction on a component and a full structure level, such as interlayer adhesiveness characterization; (4) Conduct structural components and scaled structural system moon surface environmental characteristics via experiments and 2D modeling; and (5) Effect of extraterrestrial severe environments on the materials curing process, thermal, and mechanical behavior. Upon characterizing the

relative contributions to the overall additive construction and environmental deterioration, these parameters will be calibrated to the observed experimental responses utilizing AI optimization techniques, to produce highly-calibrated computational models of the full-scale structural behavior (Figure 1). Sample materials to be investigated can include geopolymers, acid-base binders, polymers, alumina-silicates, Basalt-Mars-lunar regolith, and Portland cement.

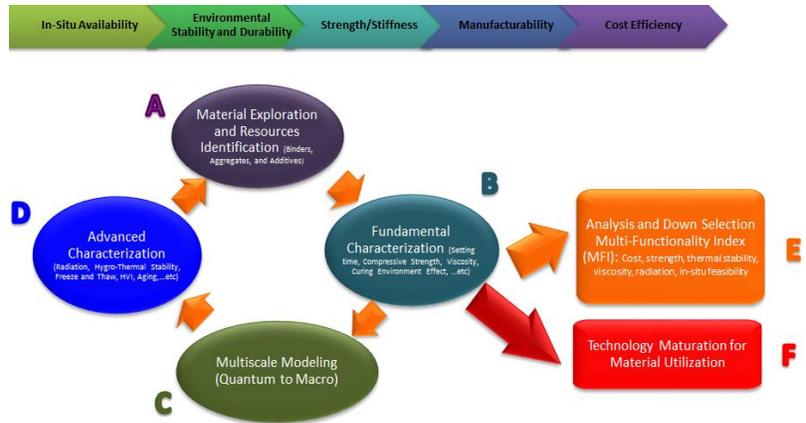


Figure 1. Technical Approach

### 1. Innovative Physics-Based Sciences for Construction Materials

**Background:** Much of the underlying science about the relationships between construction materials, processing, and the resulting properties, structure, and performance remains to be discovered for in-space construction applications. This whitepaper develops a research theme to identify, characterize, and establish aspects of in-space construction processes to provide a foundation for transformational materials research. The need for a deeper understanding of in-situ construction is rooted in materials science and engineering.

**Benefits:** Recently, additive manufacturing (AM) in the construction industry is gaining more publicity and awareness, especially for utilizing grouting materials. While research and development of concrete additive construction (CAC) are still early stages, interest in this field has been growing vastly by many private sectors and researchers. This necessitates the pursuit of a fundamental basic scientific understanding of the relationships of the material's development, technology advancement, and design of subcomponents and whole structures need to be explored and properly addressed. Hence, there is a pressing need to bridge knowledge gaps associated with transforming the advancements and accomplishments of the past century, from traditional concrete construction and material advancements to adopting revolutionary in-space additive construction technologies. This paradigm shift will require a larger leap from the researchers to transform the past material science knowledge into beneficial advancements in in-space construction roadmap.

**Examples:** While the scientific, economic, and engineering impacts are almost clear for AM applications, particularly CAC, the engineered material physical laws which drive the new materials design are still undefined. This is especially true for the performance of the final product. Research is needed to:

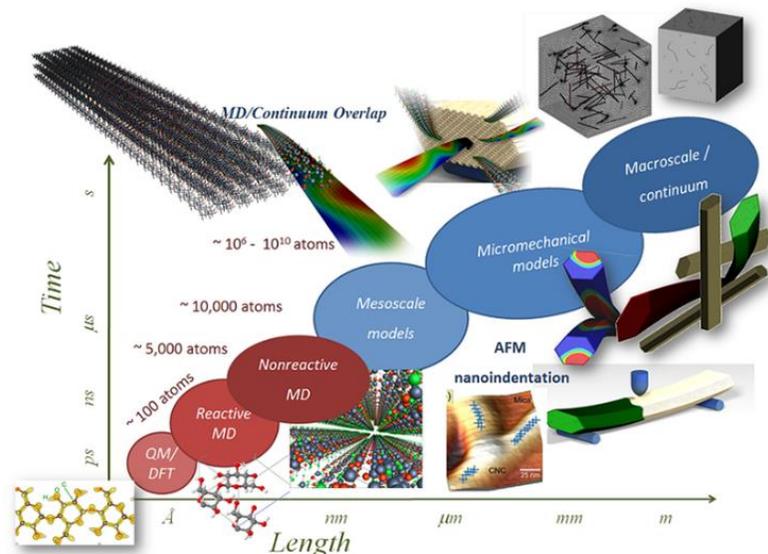
- improve and understand the capabilities of existing processes for engineering new material's, including its synthesis, characterization, and computational aspects; and the need of implementing some appropriate amendments of existing models and studies.
- generate desired biophysical sciences capabilities to advance the development of durable construction materials for in-situ AC, going beyond traditional binders, while also be extended to cement-free and Portland cement, tailored with additives as needed.
- fabricate ionic-liquid-based platforms to demonstrate in-situ binder harvesting.
- develop novel binders for multifunctional performance such as magnesia-based lunar regolith mortars and develop multiscale/multifunctional on-ground and in-space characterization schemes for synthesized binders.
- accurately measure (in situ) the regolith strength characteristics for a better understanding of its constitutive behavior in preparation for major future exploration missions.

- assess the feasibility of constructing large habitats, processing plants, and vehicle landing/ launch pads that require massive regolith excavation and hauling activities.

## 2. High-fidelity, Multiscale, Multiphysics Computational and Numerical Simulations to Predict the Physical Phenomena Underlying the Behavior of Space Materials

**Background:** NASA’s missions rely heavily on advanced space materials that can withstand harsh space, planetary atmosphere, and planetary or lunar surface environments. Moreover, there is strict weight, (multi)functionality, performance, life cycle, and reparability requirements for these space materials that render their design, development, and deployment time-consuming and costly. To accelerate the materials discovery to the deployment process, computational methods are increasingly being relied upon. These methods provide the necessary leeway by drastically reducing the materials design space, facilitating decision-making in materials selection, providing insights into the processing-structure-property-performance relationships for the said materials, and informing the experiments, thereby reducing the time and cost of experimentation. Today’s space materials are often composites, where their multicomponent nature can be exploited to tweak their functionality and properties for target performance. For example, NASA’s Computational Materials Group in the Intelligent Systems Division and Thermal Protection Materials Branch have been leading the computational materials efforts for advanced space materials such as polymers, ceramics, metals, and composites. Moreover, a roadmap has been provided for integrated, multiscale modeling and simulation of materials and systems in NASA’s Vision 2040 (published in 2018). The multiscale nature of space materials, especially composites, necessitates the utilization of multiscale, multiphysics simulation and modeling approaches to better correlate between the fundamental atomistic and molecular architecture of the materials, energetic interactions between the material constituents, and reactive or non-reactive response to external stimuli to the observed supramolecular and microscale structure and properties, and finally the material performance at the micro-, meso-, and macro scale. A schematic of multiscale composite materials modeling spanning different spatial and temporal scales is provided in **Figure 2**.

**Benefits:** Since there are innumerable combinations of matrix and reinforcement material constituents for composites, there is a critical need for the development of a comprehensive “multiscale space materials database” to serve both the computational and experimental efforts in the next decade. There are currently several materials databases developed and maintained by different NASA groups and other institutions, such as the “Materials in Space (MIS)” database, “TPSX Material Property Database,” etc. However, a “multiscale space materials database” would store a large collection of computationally generated materials data. This requires high-throughput materials simulations, especially at the atomistic and molecular levels, to provide benchmark and baseline properties of material constituents for the design of space composite materials. The computational cost of atomistic and molecular simulations using quantum, density functional theory, and molecular dynamics methods is often the



**Figure 2.** Schematics of multiscale composite materials modeling (Credit: Fernando L. Dri)

computational cost of atomistic and molecular simulations using quantum, density functional theory, and molecular dynamics methods is often the

bottleneck in these high-throughput multiscale simulations. Recently, the development of machine learning force fields (MLFFs) has drastically reduced the computational time and effort in generating materials data, bypassing the traditional time-consuming force field development efforts.

### **3. In-Space Environmental Hazards Exposure and On-Ground Testing Facilities and Validation (Cold Weather, Micro-Meteoroid Impact, Dust, Space Radiation, Microgravity, Seismic Activities, Atomic Oxygen, Vacuum, In-space Environmental Hazards Exposure)**

**Background:** In the lunar environment, thermal extremes are generally bound by the lower and upper temperatures in which hardware is expected to survive. Due to those extreme fluctuations, the long-term material's performance highly depends on emissivity changes. Thus, understanding how surface finish wear can change materials' performance over time, and how surface properties and obscuration effects (coatings) may drive materials' behavior is paramount. Moreover, collection of lunar dust via surface charging effects can cover hardware's surfaces, which may not also lead to functionality inhibition by fouling, but to wear or erosion of the coatings. A secondary offender may be the collection or buildup of molecular contamination caused by outgassing. While the causes of these interactions are generally well-understood independently, there exists a need to further develop the ground test and modeling capabilities to better understand the synergistic effects of how they impact the passive and active thermal performance of existing thermal solutions. The NASA MSFC ET V20 is currently being redeveloped as a chamber that will help answer some of these questions. With this data, it may be possible to augment the charge potential in-ground testing to better test for such effects. Future learning technologies should consider adaptive surface optical solutions combining charging-based frameworks with wear-resistant optical coatings and reflectivity control devices.

Micro-meteoroid impacts are a common hazard that should also be considered. Thus, there should be modular self-healing panel solutions in development with features such as self-identifying damage, damage scoring, reporting, and AI prioritization to ensure the safety of sensitive hardware and personnel due to meteoroids. This technology will be critical for not only the lunar surface but any other targeted space destination. The NASA MSFC Space Environmental Effects team can perform impact studies in a vacuum with the ability to support in-situ ops of active impact shielding technology concepts. Furthermore, the lunar dust hazard is a problem for mechanical moving parts, seals of all kinds, and for passive thermal solutions, but it is an even greater biohazard that needs study to enable long-term sustainable human presence. Filtering and cleaning solutions are to be found and compared to In-situ Resource Utilization (ISRU) solutions related to both extraction techniques and processing environmental safety. NASA MSFC has labs that study tribological and surface effects, optical property changes in the atmosphere, and vacuum environment.

**Benefits:** Future space exploration and building habitats are also dependent on adequate radiation shielding from the space's harsh environment. Besides meteoroids and space debris impact, the effect of cosmic rays is also an important part contributing to the harsh conditions. The space radiation hazard is most significant due to its damaging effects on biology, materials, and electronics. There is no perfect solution to space radiation that currently exists within our materials capabilities. However, studies should be made combining and optimizing existing shielding and detection technologies. In this area, AM could prove most beneficial in yielding hybrid, multi-layered structures that combine electromagnetic field generating coils and conductive networks arranged to attenuate the field using the Halbach effect. This should be a modular design that would be most beneficial as an inner layer of a habitat design. It should also incorporate on the backside of the hybrid panel a range of detection solutions that both communicate to central control to alert personnel on the shielded side of the hardware. In addition to radio and microwave radiation, cosmic rays contain high-energy particles and waves (e.g., beta, alpha, proton, atomic oxygen, ions, UV-rays, X-rays, Gamma-rays), which are to be shielded and/or dissipated via other means utilizing thermally conductive and high-density composite layers incorporated in the same structure. Since evaluating the effect of space environment utilizing space (e.g. ISS) or ground (e.g. The High Intensity Solar Environment Test system (HISSET) at MSFC) test facilities are not always available and may come with a high price tag, there is a need to develop physics-

based and phenomenological test facilities and test procedures that can mimic the impact of space harsh environment on potential space construction materials in simplified, affordable, and scaled down ground test procedures (e.g. accelerated aging or simulated high energy particle waves and hyper velocity impact and any coupling effect that may exist).

#### **4. Optimizing Large-Scale Construction Technologies and Processes to Address Biophysical and Material Sciences Related Challenges (Pore Formation, Interlayer Adhesion, Reduced Mobility, and Reduced Gravity Effects)**

**Background:** Autonomous construction advancement has been slower than any AM field, due to several challenges which could be categorized under several main areas, such as unsuitability of the available fabrication technologies for large-scale products, limitations of the materials that could be utilized by automated systems, expensive equipment, large structures stabilization, and altering material properties to deliver the expected durable performance from in situ resources to minimize the materials transport efficiency in space and cost. Severe environments such as war zones, north and south poles, equators, relief natural disaster areas, and ultimately planetary colonization by 2030 are pressing and demanding extreme environments research areas. According to the 2015 NSF 3D printing workshop report titled “Multiscale/3D printing cement” held in Vanderbilt University, some of the top challenges that the participants have identified are: (1) the rheological, hydration rates, and gelation transformation of the 3D printed binders, (2) interfacial layer adhesion, (3) deposition rate and scale relations, (4) reinforcement inclusion, (5) advancing 3D printing technologies, (6) developing new binders and modifying traditional existing ones, to adapt to the new technology transformation, (6) presenting hierarchal design strategies to link between the cementitious formulations and the additive manufacturing technologies aided by multiscale simulations. Among these challenges and others, the highest priorities were the top two in the list. There is a critical demand to expedite the transformation of in-space rapid prototyping.

**Benefits:** This task will focus on the delay between the early discovery of AC suitable binders and the ramp-up from laboratory evaluation to full-scale, in-space infrastructure implementation. Materials design and process development must be greatly accelerated to deliver timely solutions to important national infrastructural needs, such as strengthening our existing systems, reducing environmental impacts and threats.

#### **5. Artificial Intelligence and Data Analytics for NASA’s Preliminary, Ongoing, and Future Studies**

**Background:** Although science and engineering have always provided models for developing new materials and processes, recent breakthroughs in materials modeling, theory, high-throughput computation, and data mining can be exploited to significantly accelerate the discovery and deployment of advanced materials, while decreasing their cost. Growth in materials characterization, modeling and simulation, and data analytics is underway; these new capabilities require continued support to realize the potential of the development of advanced materials for in-space manufacturing.

**Benefits:** The sensitivity of the developed materials response may be established through a parametric evaluation of physical and environmental parameters to address CAC under extreme conditions, including (1) Multiscale (atomic to macro) mechanics response via simulations and experiments; (2) Materials ultimate strength rate development; (3) Structural health monitoring during and post-construction on a component and a full structure level; (4) Interlayer adhesiveness characterization; (5) Structural components and scaled structural system environmental characteristics; and (6) The effect of mimicking the severe environments on the materials curing process, thermal and mechanical behavior. Upon characterizing their relative contributions to the overall additive manufacturing and environmental deterioration, these parameters can be calibrated to the observed experimental responses in a multifunctionality optimization technique, to produce highly-calibrated computational models of the full-scale structural behavior. **Examples:** *Design of Experiments, Spectrum Reconstruction and Data Mining, Artificial Neural Networks (ANN), and Optimization and down selection Formulate a multi-functionality index (MFI) to assist in the down-selection process.*

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