National Aeronautics and
Space Administration

# Overview of “NASA Biological and Physical Sciences (BPS) Reduced Gravity and Microgravity Integrated Computational Materials Engineering (ICME) Study Final Report”


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BPS

Biological & Physical Sciences

Abstract: *NASA's push for advanced materials and processes in space and terrestrially, as captured in the latest National Academy of Sciences Decadal Survey on Biological and Physical Sciences Research in Space has underscored the need for BPS engagement with the ICME community. BPS and its predecessors have sponsored extensive flight and ground experiments yielding benchmark datasets including thermophysical properties and solidification. An overview is provided of a recent report highlighting critical research areas such as meso-scale bridging to grain-structure and coupling of fluid flow and solidification where benchmark materials science experiments conducted in the quiescent and microgravity environment are case studies. Rapid improvements in compute power and diversity are enabling linked simulations from micro- through mesoscale. A variety of accomplishments and findings resulted from this confluence of academia, industry, and government experts. The recommendations of the report provide a path to pursue ICME as an evolution of BPS projects.*

## *NASA Biological and Physical Sciences (BPS) Reduced Gravity and Microgravity Integrated Computational Materials Engineering (ICME) Study Final Report*

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# Motivation

To focus NASA Biological and Physical Sciences (BPS) Division's engagement within the broader Integrated Computational Materials Engineering (ICME) community to understand the phenomena underlying material processing, structure, and properties in the microgravity environment of space and to thereby support future space exploration efforts.

- ICME-relevant disciplines covered
  - Thermophysical properties, solidification kinetics, coupled solidification-fluids, and structures up to the grain length scale (mesoscale).
- Approach
  - Survey the heritage & current flight experiments, current ICME engagement, and future opportunities concentrating on the BPS-relevant fields of thermophysical properties, solidification kinetics, coupled solidification-fluids, and structures up to the grain length scale (mesoscale).
- Emphasis
  - The emergence of additive and in-space manufacturing gives emphasis to studies of rapid solidification in metal alloys.

Uncertainty reduction via validation datasets is a raison d'etre for microgravity materials science – generating theory and physically validated computational models useful for understanding materials both in space and on the Earth.

# Validating models by experimental flight datasets

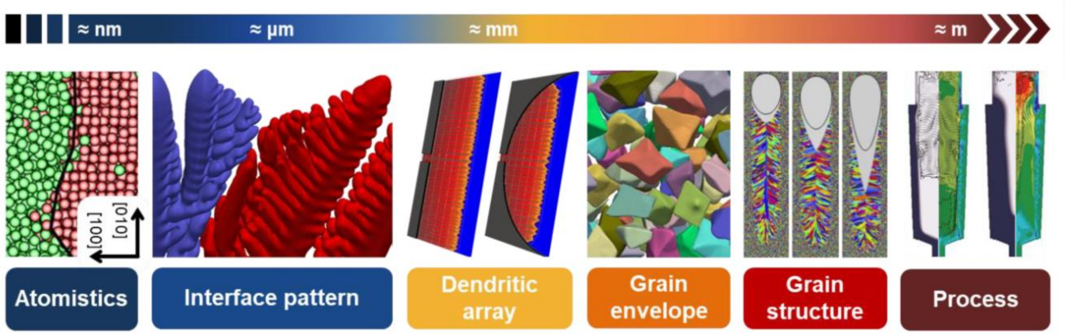
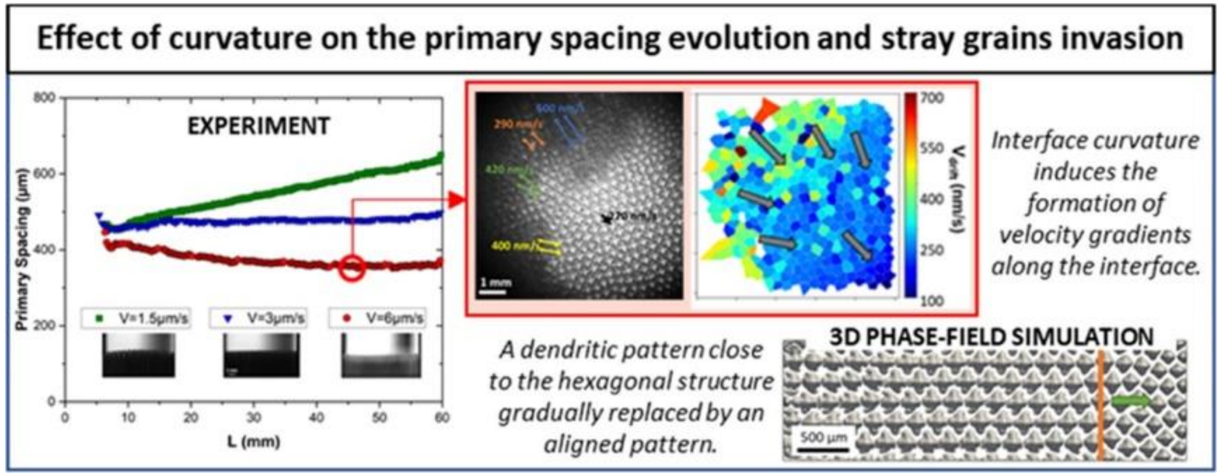
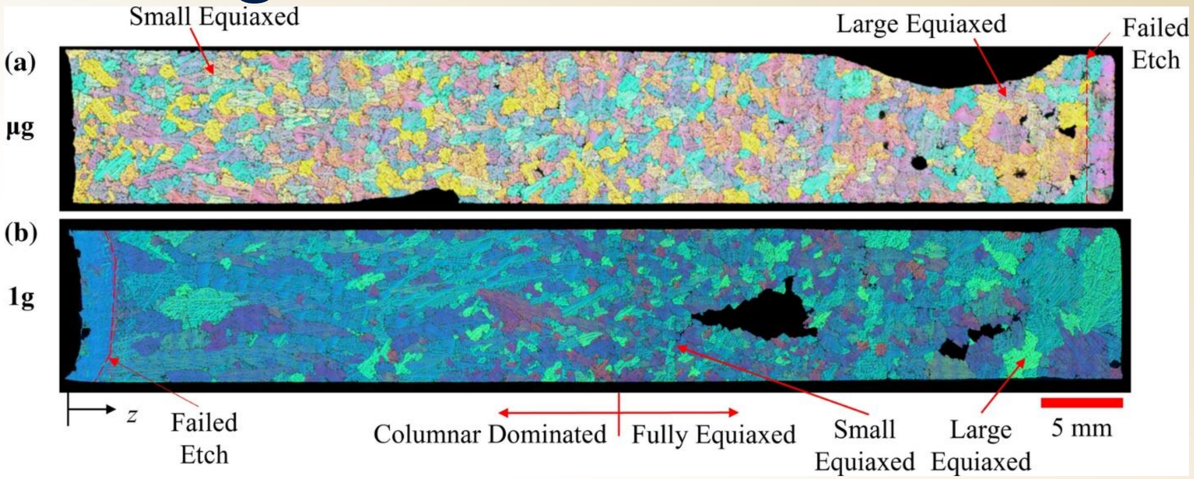



*Figure used with permission.*



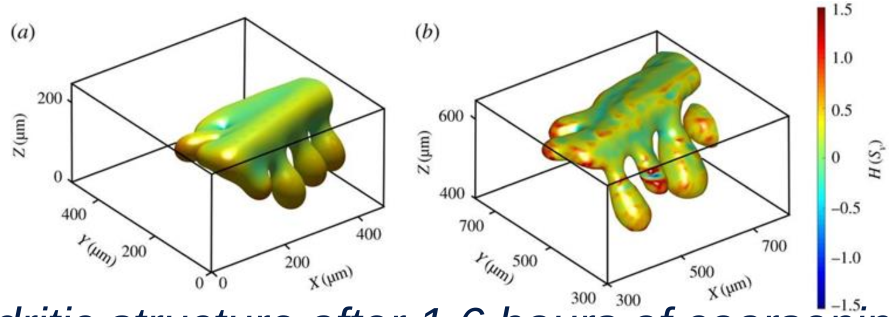

*Lacking appreciable gravitational forcing and therefore buoyancy and sedimentation within a liquid or solid-liquid mixture, flight experiments provide a clearer view of fluid-solidification coupling.*

*Figure from F. L. Mota, K. Ji, L. S. Littles, R. Trivedi, A. Karma, and N. Bergeon, "Influence of macroscopic interface curvature on dendritic patterns during directional solidification of bulk samples: Experimental and phase-field studies," licensed under CC BY-NC-ND 4.0.*



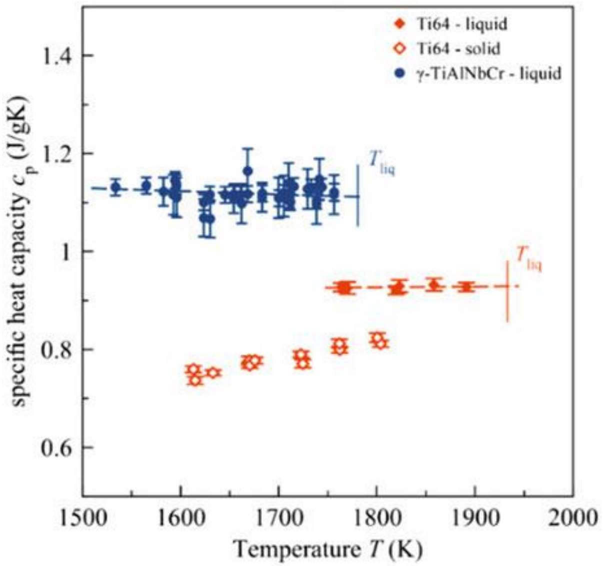

*Optical micrographs of etched aluminum-4wt%Cu specimens solidified under a) microgravity and b) 1 g in SUBSA-CETSOL.*

*Used with permission from T. J. Williams and C. Beckermann, "Benchmark Al-Cu Solidification Experiments in Microgravity and on Earth," Metall Mater Trans A, vol. 54, no. 2, pp. 405–422, Feb. 2023, Springer Nature, doi: 10.1007/s11661-022-06909-6.*



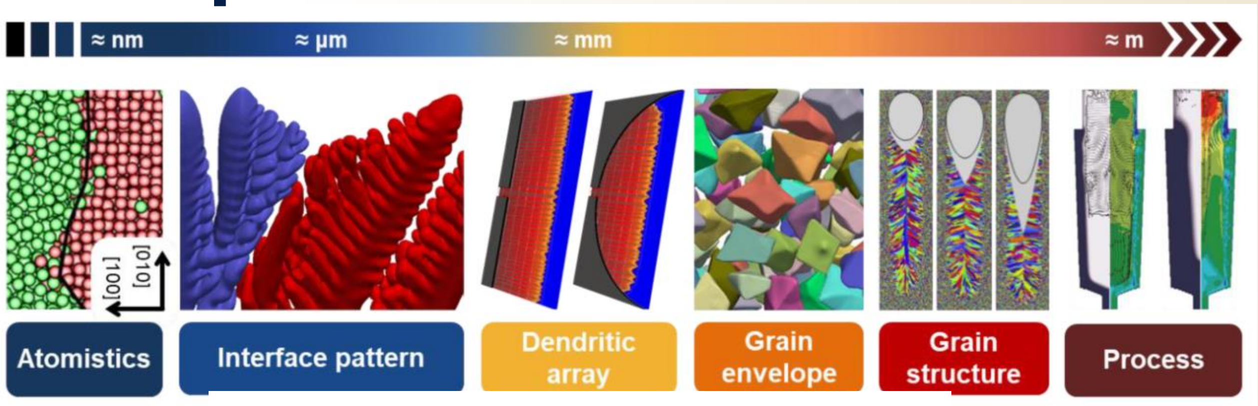

*Dendritic structure after 1.6 hours of coarsening seen a) as simulated and b) as measured experimentally.*

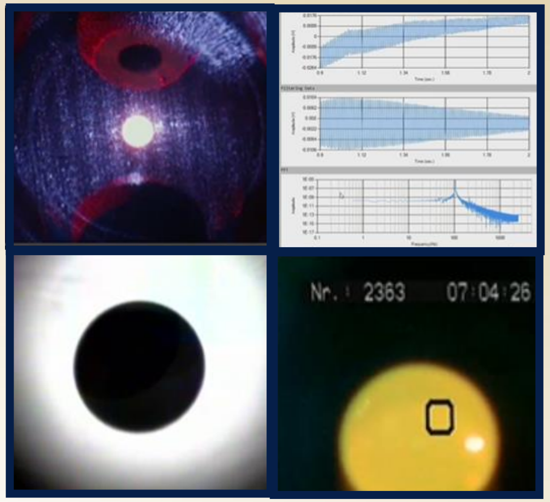
# Thermophysical Properties



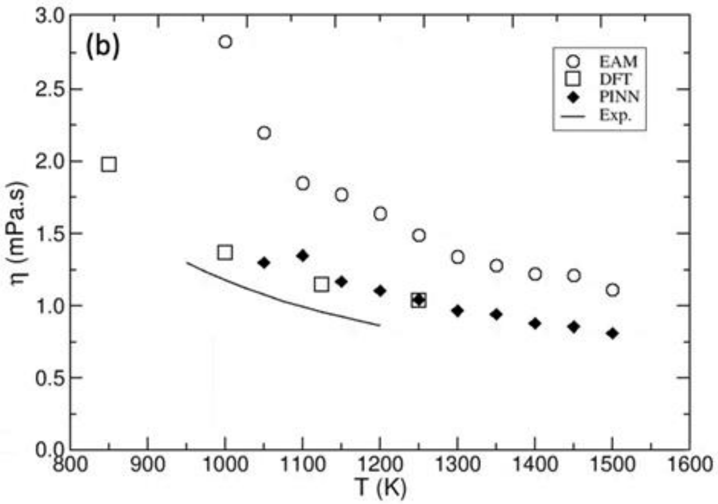

*Thermophysical properties determined through containerless levitation processing in space.*

*Figure from M. Mohr et al., "[Electromagnetic levitation containerless processing of metallic materials in microgravity: thermophysical properties](#)," licensed under [CC BY 4.0](#).*



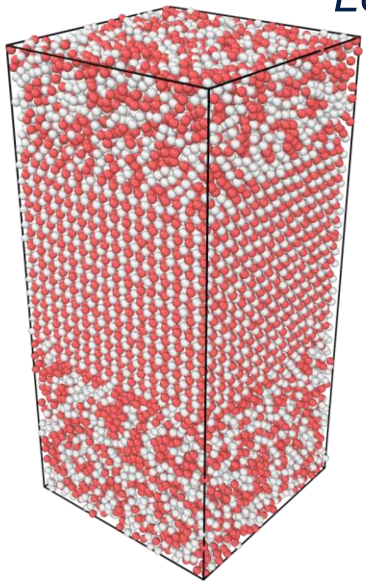




*Example of sample processing in the JAXA Electrostatic Levitation Furnace.*



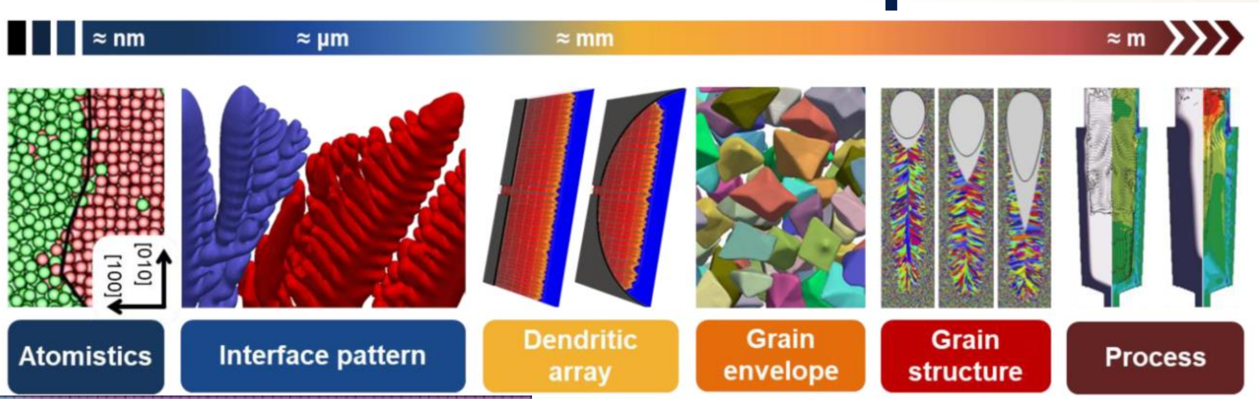

*The physically informed neural network (PINN) derived potential allowed the calculation of the energy of the liquid-solid interface, which has never been measured experimentally or calculated through the DFT method.*

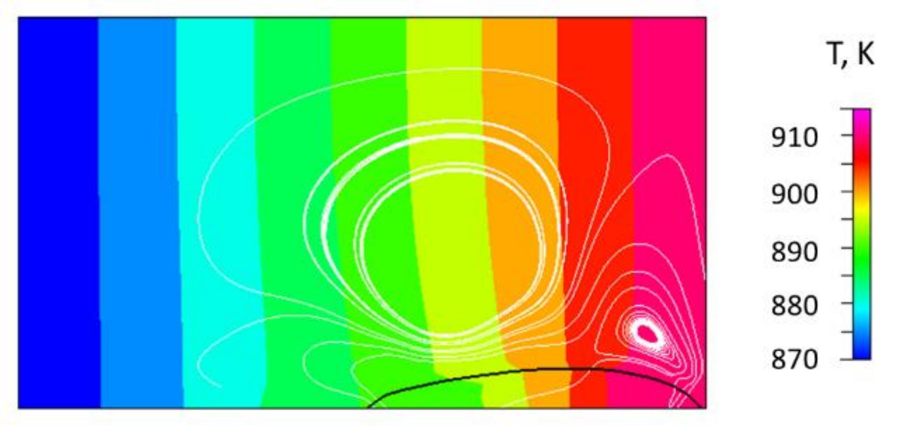
*Figure used with permission.*



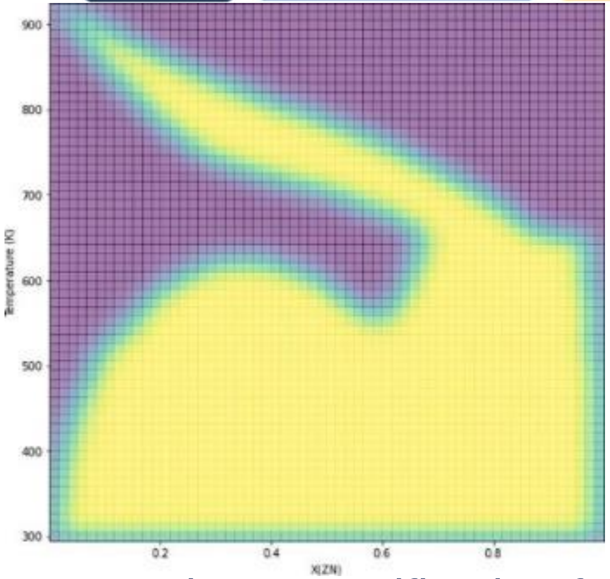
*Predictions of thermophysical & interfacial properties*

# Solidification: Next Steps



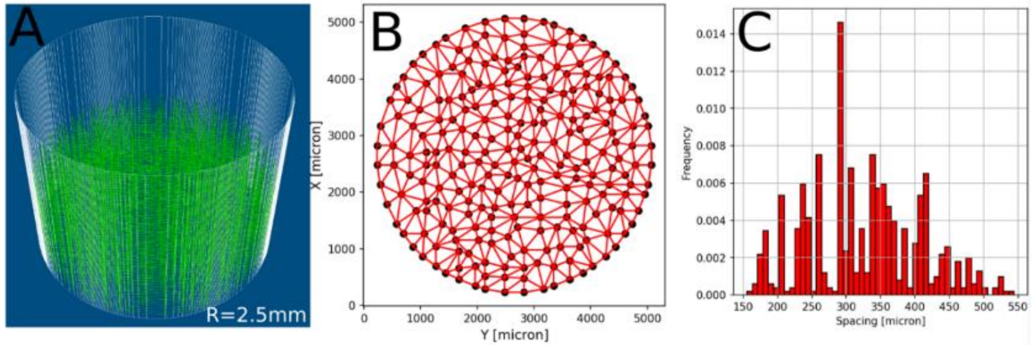




*Solidification-fluid flow coupling*

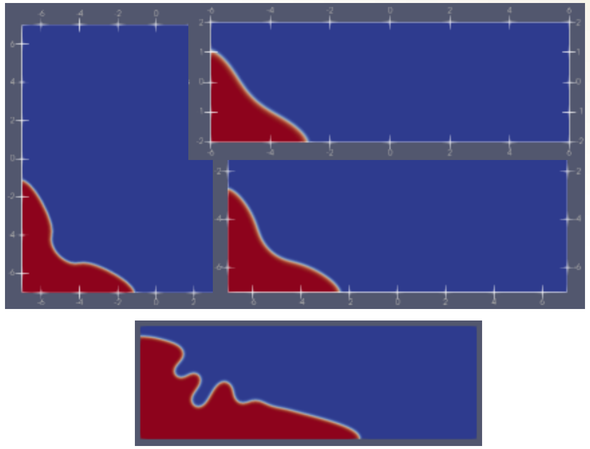



*Uncertainty quantification for CALPHAD.*

Figure from R. Otis, “Uncertainty reduction and quantification in computational thermodynamics,” Computational Materials Science, vol. 212, p. 111590, Sep. 2022, doi: [10.1016/j.commatsci.2022.111590](https://doi.org/10.1016/j.commatsci.2022.111590) with permission from Elsevier.




*Dendritic Needle Network for scale bridging*



*Comparison of MOOSE (top) and PRISMS-PF (bottom)*

# Achievements of the BPS ICME Team

**Accomplishments to Date:**

- Convened experts from academia, Agency, & industry; across all length scales from atomistic to macroscale; computational and experimental backgrounds
- Produced survey report describing flight experiments and BPS unique capabilities & role in broader ICME context
- Exercised BPS-supported academic research codes validated with BPS flight datasets and benchmarked against open-source or commercial codes widely used in ICME community
- Interacted with developers of open-source codes (PRISMS-PF, MOOSE); yielded extensions of codes – alternate formulations that support validation datasets, treadmill simulation, and 3-dimensional capability
- Implemented 2-dimensional & 3-dimensional PRISMS-PF (CPU-bound) and GPU-PF (GPU-bound) on NAS
- Published the final report as a NASA Technical Memorandum

**Findings to Date:**

- BPS datasets are foundational anchoring/benchmark datasets used to validate modeling efforts
- Interaction with code developers using BPS/microgravity datasets for validation is critical for continued progress
- Generation of useful meso/macro-scale property models via scale bridging requires accurate, precise thermophysical properties and solidification- & fluids-coupled models
- Computational infrastructure is rapidly evolving from CPU-bound to GPU, increasing throughput and enabling increasingly useful modeling efforts.
    - Moving from multi-GPU on single CPU node to multi-GPU on multiple CPU nodes for massively parallel computing that enables simulating entire sample volumes
- Models can be made relevant to industry by reducing uncertainty
    - Uncertainty quantification requires knowledge of relevant model inputs and parameters; the identification of which requires flight experimental data

# Recommendations made to BPS management

**Recommendations:**

- Accelerate flight experiments to collect critical validation datasets to:
  - Quantify and drive down uncertainty in inputs and models for engineering-relevant data to:
    - Validate materials property and processing computational and theoretical models
    - Conduct materials property and processing experiments unique to microgravity
    - Enable progression of experiments from ground to parabolic to suborbital to on-orbit
  - Champion “Can Do” science with existing ground and flight facilities and hardware
  - Investigate rapid solidification, concentrated alloys, multicomponent engineering alloys, etc. to close science gaps and reduce uncertainty via anchoring datasets
  - Engage with STMD and ESDMD to identify "experiments of opportunity” such as welding flight experiments that involve rapid solidification
  - Identify facilities requirements for future experimental platforms (i.e. CLDs)
- Invest in human capital and computational resources via:
  - Contribute to and leverage open-source codes
  - Become a visible and trusted partner in the ICME community
    - Continue engagement with MOOSE and PRISMS-PF developers
    - Continue simulation comparison using flight datasets and BPS-supported research codes
  - Support the transition of legacy codes to modern architectures with enhanced capabilities and ease-of-maintenance (e.g. CPU-bound to GPU-bound, multi-GPU multi-node)
  - Explore opportunities to employ cognitive (i.e. AI/ML) computing rather than traditional algorithmic (von Neumann) computing
  - Support/mentor research teams across multiple academic partners and NASA Centers

# Concluding Remarks

- This report can be found at the following link:
  - https://ntrs.nasa.gov/citations/20250000717
- Planning an ICME Committee meeting at American Society for Gravitational and Space Research (ASGSR) 2025
  - December 3-6, 2025
  - Phoenix, AZ
  - https://asgsr.org/asgsr-2025-phoenix/


# Thank you!