National Aeronautics and
Space Administration

NASA BPS Reduced Gravity Integrated Computational Materials Engineering (ICME) Study Results and Path Forward

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BPS

Biological & Physical Sciences

Abstract: The Biological and Physical Sciences (BPS) Division of NASA's Science Mission Directorate (SMD), and its predecessors, has sponsored extensive flight and ground experiments yielding benchmark datasets in many materials science research areas including thermophysical properties and solidification microstructure formation and evolution. The subject study sought to motivate and focus BPS's engagement within the broader Integrated ICME community to understand the phenomena underlying material processing, structure, and properties in the microgravity environment of space and to support future space exploration efforts.

BPS-relevant physical phenomena including solidification kinetics, coupled solidification-fluids, and solidification microstructures up to the grain length scale (mesoscale) are critically needed to benchmark computational models that can enable rapid advances in materials for both terrestrial and space use – for example, through better predictions of in-space joining, welding, and additive manufacturing. Leveraging the wealth of experimental data obtained to anchor incipient advances in Artificial Intelligence and Machine Learning (AI/ML) is a vital link towards efficient attainment of exploration goals. The computational means are finally becoming available to accurately model the complex (and inherently multi-discipline) phenomena involved in solidification. Making the most of the current and potential validation datasets available has never been more important.

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

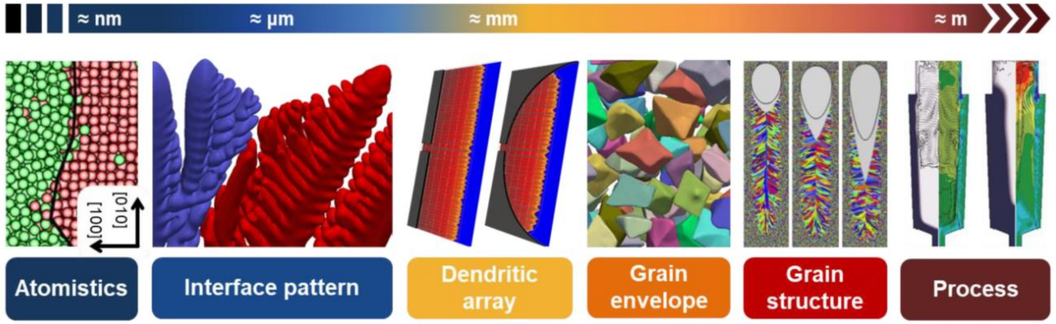
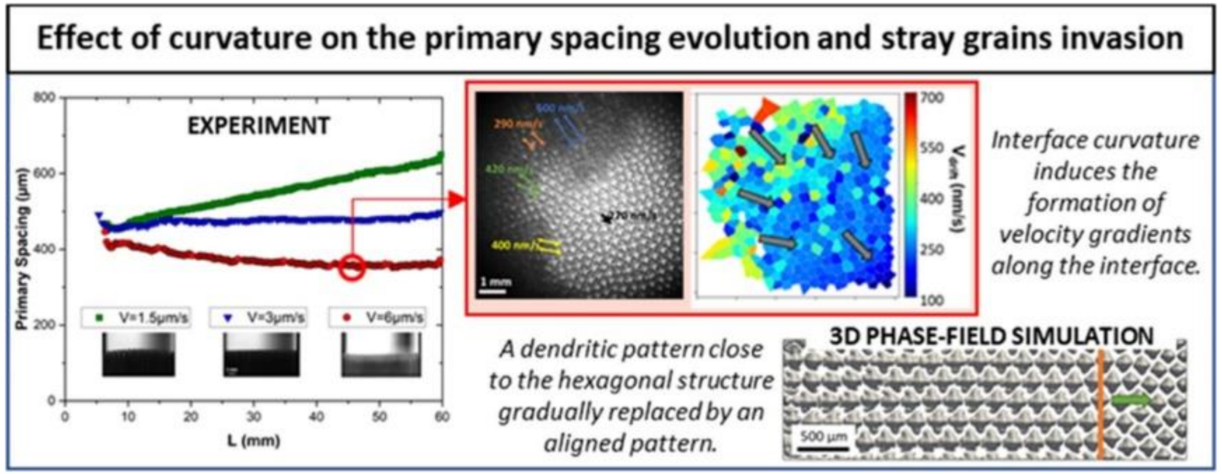
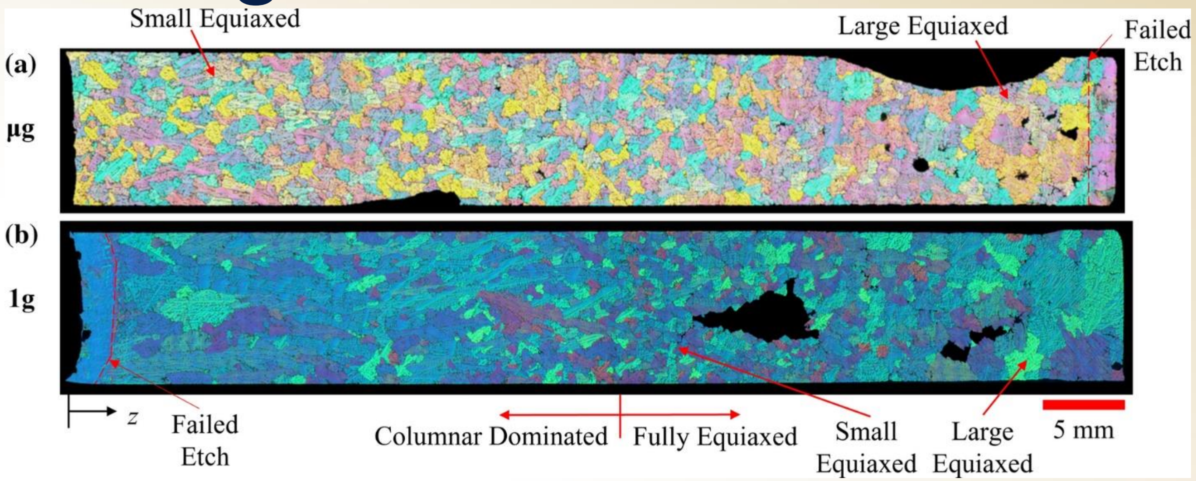


Figure used with permission.



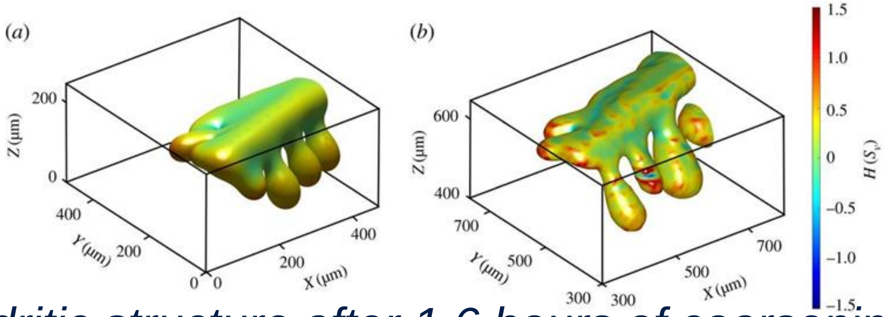
Lacking appreciable gravitational forcing and therefore buoyancy and sedimentation within a liquid or solid-liquid mixture, flight experiments provide a clearer view of fluid-solidification coupling.

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.



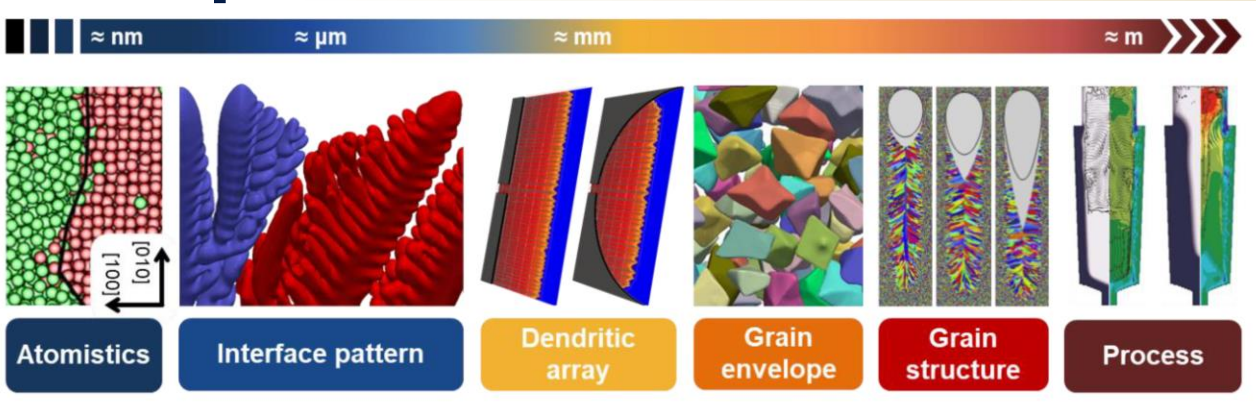
Optical micrographs of etched aluminum-4wt%Cu specimens solidified under a) microgravity and b) 1 g in SUBSA-CETSOL.

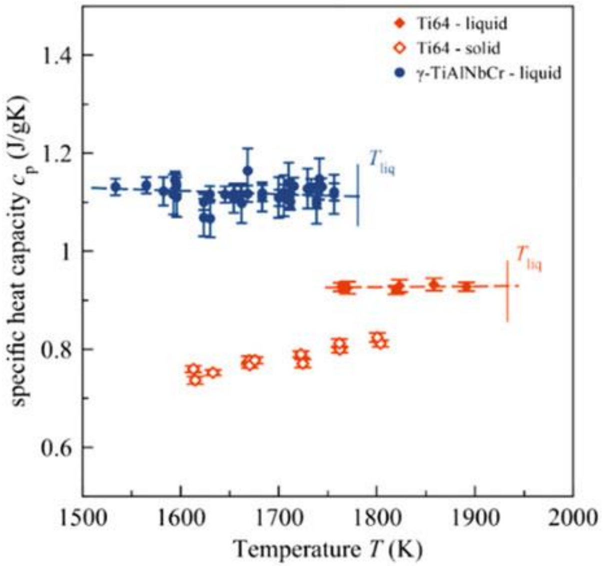
Used with permission from T. J. Williams and C. Beckermann, "Benchmark Al-Cu Solidification Experiments in Microgravity and on Earth," Metall Mater Trans A, vol. 54, no. 2, pp. 405–422, Feb. 2023, Springer Nature, doi: 10.1007/s11661-022-06909-6.



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

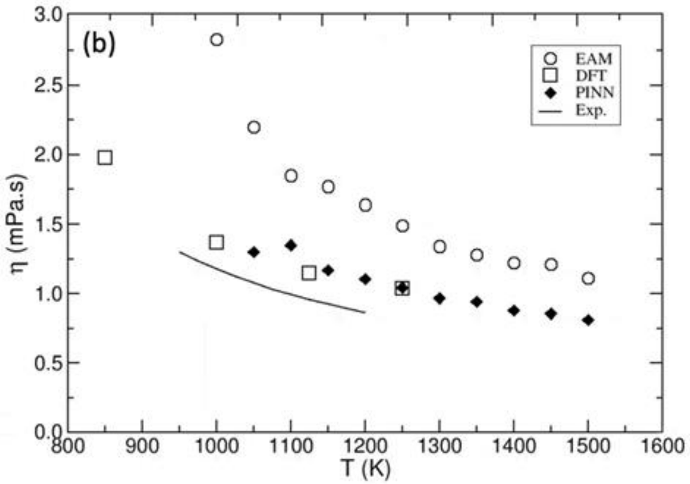
Thermophysical Properties





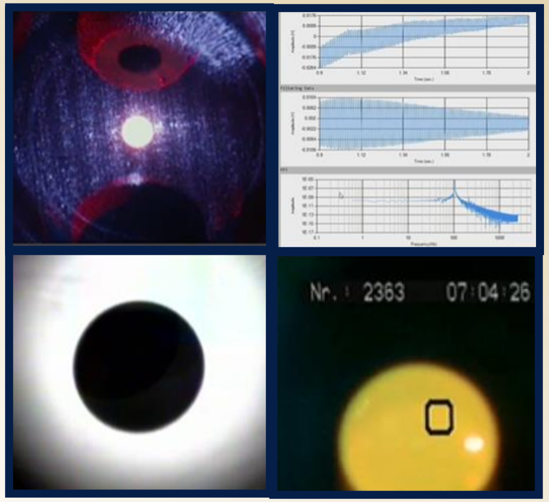
Thermophysical properties determined through containerless levitation processing in space.

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

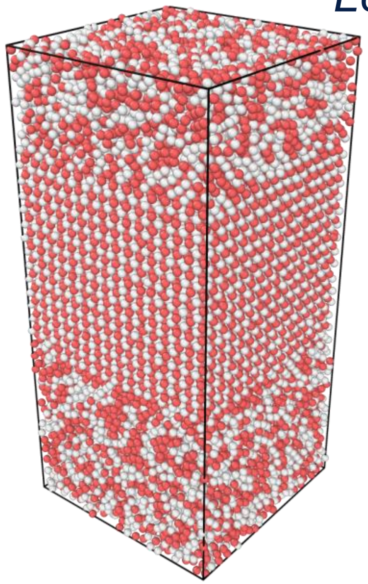


The physically informed neural network (PINN) derived potential allowed the calculation of the energy of the liquid-solid interface, which has never been measured experimentally or calculated through the DFT method.

Figure used with permission.



Example of sample processing in the JAXA Electrostatic Levitation Furnace.



Predictions of thermophysical & interfacial properties

Achievements of the BPS ICME Study Team (as of report delivery 12/2024)

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

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

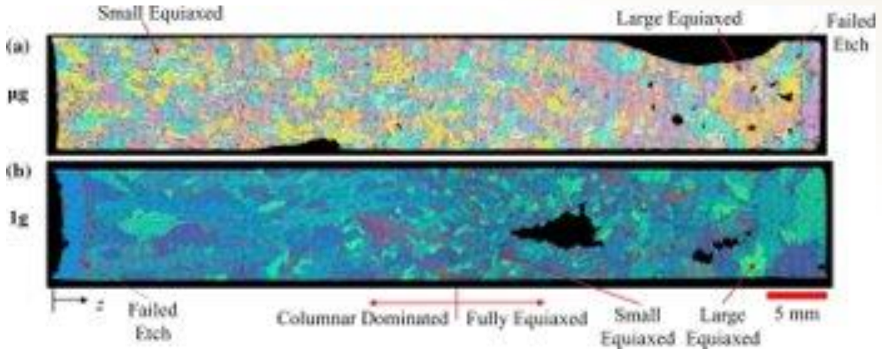
Recommendations made to BPS management

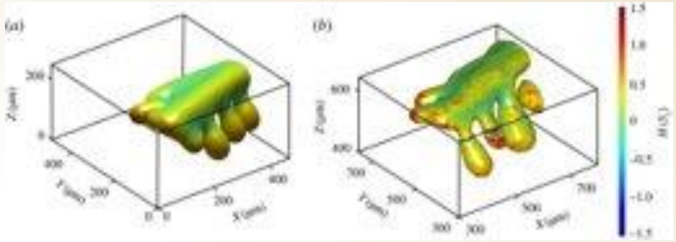
Recommendations:

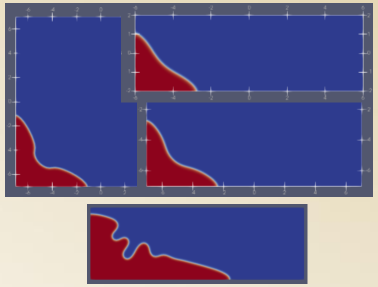
- Accelerate flight experiments to collect critical validation datasets to:
  - Quantify and drive down uncertainty in inputs and models for engineering-relevant data to:
    - Validate materials property and processing computational and theoretical models
    - Conduct materials property and processing 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

2025 Focus: Validating models/codes using experimental flight/ground datasets

- *CETSOL*
- *DFM*
- *DECLIC-DSI*
- *MICAST*
- *PFMI*

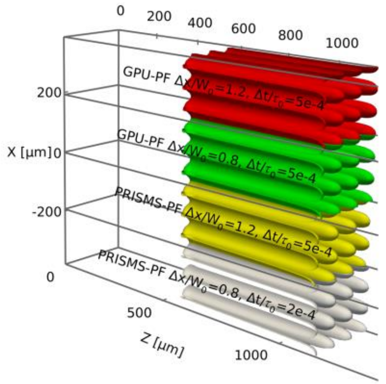






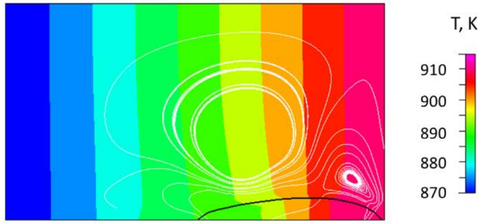
Comparison of MOOSE (top) and PRISMS-PF (bottom)

Benchmarking state-of-the art PF solidification codes

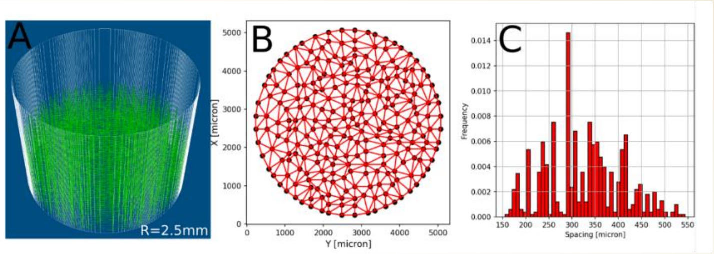


Solidification-fluid flow coupling

Image from ICME Report, CFD-ACE+ Simulation



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)



Dendrite Needle Network model evolution supports scale bridging and fluid flow coupling

Connection to Applied Exploration Projects:

- ***ESI24: CME for Lunar Metals Welding***
  - ***Weld-ASSIST Weldability Assessment for In-Space Conditions using a Digital Twin***
  - ***P-S-P Linkage of Lunar Metal Welding with Internal Defects***
- ***SBIR Ignite! PY25 ICME Subtopic***

NASA/MSFC/EM31 In-House Modeling Status:

- *Phase Field & 2D DNN models on NAS: simulations & post-processing underway*
- *Flow 3D Cast Module + Flow 3D AM Module validation studies imminent (funding dependent) – tied to ongoing and proposed work in weld, cast, AM*
- *2D-DNN – flow model (research code) being provided through SME*

2025 Dissemination/ 2026 Plans

- TM version of report can be found at the following link:
  - https://ntrs.nasa.gov/citations/20250000717
- Two presentations at TMS ICME 2025:
  - Overview of "NASA Biological and Physical Sciences (BPS) Reduced Gravity and Microgravity Integrated Computational Materials Engineering (ICME) Study Final Report" (presented by Peter Voorhees)
  - "Benchmarking Massively Parallel Phase-Field Codes for Alloy Solidification" – J. Tian and A. Karma: Northeastern University (co-authors D. Montiel, J. Landini, K. Thornton: PRISMS-PF group Univ. Michigan)
- 7th International Conference on Advances in Solidification Processes (ICASP-7)
  - Plenary lecture " Phase-field modeling of far-from equilibrium solidification processes: from additive manufacturing to ice templating" – A. Karma
  - Microgravity Solidification, faceted interfaces and intermetallics, fluid flow sessions
- ICME Path Forward Discussion at American Society for Gravitational and Space Research (ASGSR) 2025
  - Following this session, same room
  - https://asgsr.org/asgsr-2025-phoenix/
  - Ad hoc group to meet in near-term to regroup beginning with this discussion
- 2025 MRS Fall Meeting: (topical cluster) MATERIALS THEORY, COMPUTATION AND DATA SCIENCE (MT)
  - Symposium Sessions | 2025 MRS Fall Meeting & Exhibit | Boston, Massachusetts
  - Nov 30 – Dec 5, 2025
- 2026 TMS Annual Meeting
  - Materials Research in Reduced Gravity Symposium (Organizers:Sillekens; Sansoucie; Hyers; Matson; Bracker; Ishikawa) SYMPOSIUM ABSTRACTS
    - NASA's Biological and Physical Sciences (BPS) Reduced Gravity Integrated Computational Materials Engineering (ICME) Study – Littles & al.
    - Laser Beam Welding Benchmark Experiments Performed in Reduced Gravity and Vacuum – O'Connor & al.

BPS

PSI Analysis Working Groups (AWG)

- **2026 VISION:** Replicate for the physical sciences, what OSDR has accomplished for biological sciences with their OSDR AWGs.
- AWGs are intended to be *community-lead*, distinct from PSI, with supplementary guidance available from NASA researchers.
- Membership is open to all experience levels with participation being voluntary.

Objectives:

1. Enable collaboration & reuse of data for additional scientific discovery, including new proposal development.
2. Increase the dissemination of results from data available in PSI.
3. Facilitate data organization & analysis.

- An AWG for each physical science research area is expected for a total of six.
- First AWG kick-off estimated by Jan. 2026 & focuses on *Combustion Science*.

Scan to request to join.

Thank you!