

FY23 LDRD Calls & Research Needs

Thank you for your interest in the Sandia National Laboratories LDRD program! Each program area below contains a description of the program, along with high-level research needs. Please use the form linked in the email to submit your research summaries that align with the program areas below. Each research need contains a unique identifier that you will use a key to select on the form. You may select more than one area per submission. Contact academicprograms@sandia.gov with any questions.

Bioscience (Bio)

The Bioscience Research Foundation (RF) performs R&D required to anticipate, detect, and counter the risks of natural and man-made biothreats (biodefense) and to mitigate the impacts of climate change by advancing scientific understanding and developing technological solutions (environmental security). In the area of Biodefense, we address both natural and man-made biological agents, digital biosecurity, and materials, which can be either enabling or a target for manipulation. In the area of Environmental Security, we address the impacts of global climate change, bioresource security, and the need to drive the circular bioeconomy.

To focus RF efforts in biodefense and environmental security, we have identified three thrusts in each area. In Biodefense, these are Anticipatory and Threat Science, Detection and Diagnostics, and Countermeasures. The Environmental Security thrusts are Predictive Biology, Biosystem Design, and Controlling Carbon Flux.

Needs:

BIO1:

Applications of virology, predictive biology, or microsystems to leap ahead in pandemic preparation and response

BIO2:

Investigations of the biological implications of climate change

BIO3:

Applications of predictive biology tools to biomanufacturing using non-traditional chassis and to climate change

BIO4:

Advances in the production of sustainable aviation fuels from alternative feedstocks

Computing and Information Sciences (CIS)

The overarching goal of the CIS IA is to deliver innovative R&D that significantly advances computing and related sciences for the full spectrum of Sandia missions. The scope includes computer and computational science and engineering (including high-performance computing and computing architectures), information and data science, computational mathematics, and artificial intelligence. In all cases, CIS R&D must have a line-of-sight to impacting Sandia's current and/or future missions.

Needs:

CIS1:

Trusted Artificial Intelligence:

Mathematical foundations of Artificial Intelligence (AI) and Machine Learning (ML) that quantify uncertainty, improve explainability, and provide resiliency to adversarial subversion.

CIS2:

Mission-Driven Computing Co-Design:

Co-design across computing systems, software, operations, algorithms, and applications to enable the complex workflows demanded by future mission applications.

CIS3:

Empowering Humans through Computing:

Workflows, automation, decision support, and human-data systems that improve productivity and enhance our ability to design national security systems.

Earth Sciences (ES)

All national security challenges have some intersection with earth science. Sandia's missions focus on the scientific and engineering aspects of national security. The Earth Science Research Foundation (RF) emphasizes "Quantitative Earth Science for National Security." The intersection of national security and Earth Science occurs across a wide zone spanning tens of kilometers above to several kilometers below the earth's surface. Across this wide zone encompassing the solid earth, oceans, and the atmosphere, Sandia's Earth Science R&D must address the coupled thermal, chemical, biological, hydrological, physical, energy propagation, and mechanical behavior of naturally occurring, significantly heterogeneous, and dynamic materials, ensuring integrated understanding and information across scales ranging from nanometers to hundreds of kilometers. Quantitative elements include detailed characterization, data analytics, and machine learning applied to both interpretation and simulation, new numerical techniques, and all forms of modeling. For FY23, the Earth Science RF will continue its focus on research problems at the intersection of climate change and national security. Talent pipeline development is also a priority, so university partnerships with student and postdoc engagement in projects are strongly encouraged.

Needs:

ES1:

Sensing tools and methods that provide multi-dimensional (space, time, types of data) information

ES2:

Tools for mapping and integration of complex data streams and for deriving meaning from large data sets relevant to the Earth Sciences

ES3:

Micro- to macro-scale multi-phase flow and transport modeling for earth sciences

ES4:

Approaches, models, and computational tools that provide better parameterization for Earth Science problems

ES5:

Atmospheric data collection, models, and interpretation that can explain natural and anthropogenic changes

ES6:

Data collection, models, and rapid interpretation of coastal, ice, ocean cloud, and sea floor chemistry and physics processes

ES7:

Examination of the physics and chemistry at the interfaces among various earth spheres: atmospheric, ocean, seafloor, coastal, water resources and solid earth

Energy & Homeland Security (E/HS)

The Energy & Homeland Security (E/HS) portfolio at Sandia National Laboratories secures the nation's critical infrastructures and environment against attacks, threats, and climate change by performing world-class research and development (R&D). The overlapping and dominating threat drivers of climate change, cyber, and bio steer much of the work of the E/HS portfolio. Responding to these threat drivers requires a variety of technology R&D pathways and a systems approach to creating future energy systems and protecting our homeland.

The United States relies on abundant, reliable, and affordable energy for its security, economy, and the well-being of its people. The need for climate change mitigation and adaptation will drive near- and long-term changes to both the nation's energy systems and its critical infrastructures. Increased connectivity, the use of digital control systems, and great-power competition are leading to diverse and sophisticated cybersecurity threats. COVID-19 has demonstrated that a pandemic is a national security threat as well as a public health threat. Secure and resilient solutions are needed to combat threats that may intersect energy, cyber, chemical, and biological vulnerabilities.

Engineering Science (ENGSCI)

The Engineering Sciences Research Foundation (ESRF) drives understanding and innovation by integrating theory, computational simulation, and experimental discovery and validation to elucidate and credibly predict the behavior of complex physical phenomena and systems. The ESRF provides leadership and stewardship for a set of critical technical capabilities: aerosciences, combustion/fire sciences, fluid mechanics, energetics, shock physics, solid mechanics, structural dynamics, thermal sciences and computational simulation technologies.

Needs:

ENGSCI1:

Fundamental and Coupled Physics Phenomena: discovery of fundamental, coupled physical phenomena in terms of characteristic length and time scales and development of predictive engineering science models needed to predict the as-built manufactured/assembled state performance of engineered systems. This includes discovery research and model development that span the space from defect formation phenomena during manufacturing processes to performance in service environments. Of specific interest are coupled physics and combined environment response including mechanical/thermal/radiation science use cases.

ENGSCI2:

Next Generation Engineering Simulation: discovery of algorithms and methods as well as development of efficient and accurate modeling and simulation techniques is required in the design, development, qualification and sustainment stages of complex systems, across a wide variety of length and time scales. Coupled multi-physics and multi-scale computational methods must be both efficient (including CAD-to-Solution workflow and especially meshing) and credible (including verification, validation and uncertainty quantification) to leverage the advancements afforded by the next generation of high-performance computing platforms. Additionally, hierarchical multi-resolution, multi-fidelity, or reduced-order modeling frameworks are sought which capture complex high-resolution physics phenomena and predict their effects in a credible manner with lower computational cost, paving the way beyond forward simulations.

ENGSCI3:

Diagnostics and Experimental Capabilities for Engineering Applications: discovery research and development of novel diagnostics and experimental testing capabilities are needed to capture phenomena and responses across multiple time and length scales up to and including the system level. Diagnostics that improves understanding of manufacturing processes, as-built state, and performance and validation testing are of interest as a part of an integrated engineering solution. This includes novel approaches to significantly improve production and safety experiment/testing and positively impact “cost, performance, schedule” in our engineering science applications.

ENGSCI4:

Engineering Data Integration and Interrogation: formulation and integration of data science techniques to identify/discover and extract buried knowledge/trends in massive engineering data ensembles (either experiments, computational simulation or a combination of the two) or large single data sets exhibiting extreme temporal and spatial resolution. This includes (a) techniques for validation assessment using disparate data sets, (b) improved methods for handling data sets that are noisy, includes anomalies/defects and/or missing data, (c) integration of heterogeneous observational information, simulation data, and SME opinion for key decision-making processes and (d) approaches for fusion of data and physics models that fill physics gaps and improve the predictive capabilities of the models.

Global Security (GS)

The Global Security (GS) LDRD Investment Area seeks a broad spectrum of R&D efforts that advance our ability and meet our vision to deliver innovative engineering solutions to protect the nation from strategic threats at home and abroad. The GS Investment Area is organized using two core Focus Areas: Weapons of Mass Destruction Security (WMDS) Focus Area and the Space and Remote Sensing (SRS) Focus Area.

Needs:

GS1:

Weapons of Mass Destruction Security

The WMDS focus area aims to reduce U.S. national security risks posed by weapons with the capability to create destruction and death on a massive scale. Within scope of WMD Security are the traditional categories of chemical, biological, radiological, and/or nuclear (CBRN) weapons and devices, as well as

innovative, disruptive, and/or integrated technologies that, when tied with CBRN, could present significant risks to U.S. national security interests. WMDS research interests include:

- **Unmanned aircraft systems (UAS) and counter-UAS (CUAS):** Novel detection and mitigation approaches that address the continued evolution of UAS technologies and threats.
- **Ensuring asset security:** Revolutionary approaches for physical security of assets from cradle to grave and from fixed location to mobile. Innovative approaches for remote, wireless power and communication; mobile and adaptive autonomous sensing enabling intelligent threat awareness; and novel approaches to controlling and interacting with environments within secure areas.
- **Enhancing WMD response:** Differentiating technologies for rapid identification, analysis, disablement, and attribution of WMDs (including chem/bio), decision-making tools, and materials and technologies that enable WMD response capabilities.
- **New reactor technologies:** R&D that supports assessing proliferation challenges from emerging technologies and their impact on national security, including discrimination of dual-use technologies. Analysis and quantification of safeguards and security as they pertain to proliferation including non-traditional fuel cycles and advanced reactors and small modular reactors.
- **Treaty monitoring:** Novel ideas to address complex challenges in warhead monitoring, counting, multilateral treaty compliance, denuclearization and verification, chem/bio and treaty monitoring capabilities to support climate agreements, e.g., high resolution monitoring of Green House gas emissions.
- **Quantum Technologies:** Innovative applications of quantum technologies for communications, detecting CBRN materials, assessing CBRN warheads, and securing CBRN facilities, e.g., quantum fencing.

GS2:

Space & Remote Sensing

The SRS focus area addresses unmet U.S. national security mission needs in global monitoring by investing in techniques and technologies to realize pathfinding remote sensing systems, advancing ground system technologies for mission data processing, and data fusion and exploitation to enable decision making and anticipatory knowledge generation. SRS research interests include:

- **Novel data architectures or remote sensing algorithms (detection, tracking, event and activity classification) for near-real-time multi-int fusion** leveraging remote sensing data (i.e., commercial satellites) and other disparate data sources (seismic, infrasound, other ground sensors). Multi-int fusion seeks to combine information from a wide variety of data sources to achieve analysis and decision supporting inferences that cannot be achieved with a single source.
- **New techniques or algorithms to detect low SNR targets in the presence of high intensity backgrounds.** Algorithms for asynchronous or event-based detection as well as algorithms that could be mapped to FPGAs to enable more on-board real-time processing are of particular interest.

- **Advanced sensor designs for space-based applications ranging from the ultraviolet to long-wave infrared** including components that could transform performance of space-based sensing applications (e.g., cutting edge space electronics, improved cryo-cooler concepts for LWIR, or other FPA thermal management concepts).
- **Hardware or sensor technologies that enable multi-mission capabilities** like simultaneous nuclear and non-nuclear event detection. Examples include development of multi-waveband ROICs by changing or adding an IR transducer diode layer or detector technologies that enable radiometric dynamic range over 5 orders of magnitude from a focal plane array.
- **Advancements in RF communication technology** that enable miniaturization of antenna and receiver systems for applications in low power/low SNR signal reception in contested environments.

Materials Science (MS)

MS1:

Discovery of new material systems and manufacturing processes:

- Advanced synthesis and manufacturing processes for organic, ductile, brittle, electronic, optical, and multi-materials.
- Discovery of new materials that enable advanced manufacturing capabilities.

MS2:

Materials discovery and fundamental understanding:

- New materials and interfaces with tailored properties, enhanced performance, and/or new functionality supporting Sandia mission needs.
- Resilient and self-healing materials.
- Materials with novel properties uniquely enabled by quantum effects.
- Materials to enable novel energy conversion and storage.
- Capabilities to increase understanding of fundamental material and interface degradation and failure mechanisms.

MS3:

Development of advanced measurement science capabilities:

- Novel non-destructive measurement methods that screen for critical defects.
- High throughput and/or high-fidelity materials characterization techniques (e.g., enhanced spatial/temporal resolution experimental capabilities).

MS4:

Enabling computational priorities:

- Approaches for bridging length and time scales that capture critical materials physics in engineering models with quantified uncertainties.
- Leveraging current advances in machine learning and artificial intelligence, in combination with fundamental understanding of materials science, to create new materials, processing capabilities, or accelerated understanding/characterization of existing materials.

Nanodevices and Microsystems (NM)

The NMRF IA seeks proposals that:

- Increase our understanding of physical phenomena and our ability to manipulate and control them from the nanoscale to the microscale.
- Develop innovative nanoscale and microscale devices.
- Achieve new methods of integration.
- Enable new mission capabilities through novel microsystems.

The NMRF Investment Area Team (IAT) will place priority on funding innovative scientific concepts aligned with Sandia's mission strategies and Lab Priorities.

Needs:

NM1:

Trusted resilient microsystems:

The development of concepts, devices and tools that enable the understanding and creation of Extreme-Environment-Hardened microelectronics and microsystems that are resistant to subversion. This includes proposals that further understanding of combined extreme environments impact on microsystem performance (ionizing radiation with high temperature, high power electromagnetic radiation, high shock, etc.).

NM2:

Beyond Moore's Law computing technologies:

The development of nanoscale and microscale concepts, devices, tools and systems that extend performance improvements beyond Moore's Law

NM3:

Optoelectronics of the future:

The discovery and creation of advanced optoelectronics, at the nanoscale and microscale, which provide new functionality

NM4:

Advanced Microsystem Sensor Technologies:

The development of nanoscale and microscale concepts, devices and systems that enable physical, chemical, radiation, nuclear materials, and explosives detection exceeding current limitations in selectivity, sensitivity, and/or robustness

NM5:

Nanoscale- and Microscale-enabled Performance:

The discovery and exploitation of new functionality resulting from phenomena unique to the nanoscale and microscale; this thrust seeks to invest in enabling those scale-dependent phenomena such as non-continuum and quantum

National Security Programs (NSP)

The National Security Programs (NSP) Mission Foundation (MF) funds innovative research and development (R&D) to enable trusted, threat-informed, pathfinder technologies and systems for national security applications.

Needs:

NSP1:

Cyber Innovation (CYBER)

The CYBER focus area applies science and engineering principles to understand and enhance the secure operation of complex, high-consequence national security systems in adversarial environments. We seek novel ideas that integrate end-to-end cybersecurity with the science and engineering enabling national security mission areas. Most projects fall into one or more of the following categories: cyber-physical systems, next-generation mobile/Internet of Things (IoT) technologies, quantum information technologies, and cyber science & experimentation.

Research Needs

- *Hardware systems understanding:* security & assurance from materials to computation (e.g., physics/materials effects on Physical Unclonable Function/Random Number Generator (PUF/RNG) output; signals from noisy near-field environments; extension of cryptographic security)
- *Software systems understanding:* static & dynamic analysis to characterize nominal/abnormal behavior; translation of vulnerability insights to measurements of risk; improved speed/accuracy in reverse engineering
- *Data systems understanding:* authenticity, validation, verification, & trust; streaming analysis; edge processing
- *Data analytics, machine learning:* explainable models; counter-adversarial models; new-data/existing-model compatibility; host-based telemetry; analytics left of attack

NSP2:

Heterogeneous Integration & Trusted Radiation-hardened Microsystems (HI&TRH)

The HI&TRH focus area seeks solutions to integrate diverse technology components into a higher-level microsystem assembly with improved performance and optimal space, weight, and power for trusted and/or radiation-hardened applications.

Research Needs

- Integration of separately manufactured components into a higher-level microsystem assembly that provide enhanced functionality and improved operating characteristics
- Techniques for incorporating multiple disparate technologies such as complementary metal-oxide-semiconductor (CMOS) logic and memory, compound semiconductor microelectronics and photonics, silicon photonics, micro-electro-mechanical systems devices, passive components and sub-systems
- Computing capabilities that can provide insight into effects of heterogeneous integration on TRH performance for a broad range of solution options

- New/modified integration processes that enable low-cost, low-volume, rapid R&D and prototyping efforts with a variety of technologies

NSP3:

Intelligence Science for Proliferation (ISP)

The ISP focus area seeks technologies that can be used to identify, analyze, understand, and counter threats from a range of potential adversaries.

Research Needs

- Autonomous, innovative sensing systems, and sensor integration
- Artificial Intelligence/Machine Learning (AI/ML), social system theory, data integration for strategic and operational exploitation of data

NSP4:

Radio Frequency Supremacy & Hypersonics (RFS&H)

The RFS&H focus area needs to understand the various effects of system design, components and materials on hypersonic and sensor systems.

Research Needs

- Global Positioning System (GPS)-denied navigation and control
- Advanced waveform research that enables resilient, agile processing for RF image formation, communications, autonomy, and sensor systems
- Multi-mission RF architectures using trusted electronic systems with smaller size, weight and power
- Novel tools and techniques enabling rapid, physics-based concept exploration and design optimization
- MBSE approaches for linking high fidelity EM models to effects previously only revealed via measurement

New Ideas (NI)

The New Ideas IA solicits proposals that do not fit neatly into the categories or priorities covered by the other LDRD Investment Areas.

Needs:

NI1:

Fundamental research in fields of current interest to Sandia that are outside the strategy space of the other IAs

NI2:

Research at the boundaries between IAs, interdisciplinary topics, and unconventional ideas

NI3:

Ideas that propose nascent research in an emerging new research field that may become relevant for national security

NI4:

Out-of-the-box approaches to address mission needs.

Radiation, Electrical, and High Energy Density Science (REHEDS)

The Radiation, Electrical, and High Energy Density Sciences (REHEDS) LDRD Investment Area (IA) seeks to advance the fundamental understanding of the science of nuclear weapons and their effects. This understanding is critical for the present stockpile as well as for the systems of the future as articulated in the Nuclear Posture Review. The REHEDS IA looks at four key discipline areas to advance this understanding, each of which play a pivotal role in supporting a safe, secure, and reliable stockpile that is viable today and will be robust to evolving threats and technological surprise. These four disciplines include

- *Radiation Effects Science (RES) — This discipline focuses on understanding the effects caused by single and combined radiation environments.*
- *High Energy Density Science (HEDS) — This discipline focuses on the experimental, theoretical, and computational study of material properties, radiation transport, inertial confinement fusion, and other physical processes at extreme temperatures, densities, and pressures.*
- *Electrical & Electromagnetic Science (EES) — This discipline focuses on understanding the effects of electromagnetic radiation, with a particular focus on electrical and electro-optical circuits.*
- *Pulsed Power Science and Technologies (PPS&T) — This discipline focuses on understanding the physical principles that underlie the efficient creation and application of electrical energy through pulsed power technologies.*

Needs:

REHEDS1:

Radiation Effects Sciences (RES)

Radiation effects science proposals are solicited in the following topical areas that are associated with the production/characterization of radiation environments at Sandia facilities, and the analysis of effects in electronics and materials driven by the environments.

- **X-ray environments and effects:** The most-energetic “hot” x-rays (100 keV-1 MeV) and gamma-rays (>1 MeV) are the most penetrating and can affect electronics deeper in the system, including dose-rate-driven effects such as transient radiation effects in electronics (TREE) and a class of EMP called Internal EMP (IEMP) at the sub-system and component level. A key research challenge is advancing the fundamental understanding of such dose-rate effects.
- **Neutron environments and effects:** Neutrons are encountered in both the exo-atmosphere and the endo-atmosphere. Interactions with the atmosphere cause neutron spectra to become less energetic (10 eV - 1 MeV) and to arrive in a broad pulse, thereby generating long-duration gamma radiation. Key research needs in this area are (1) Understanding the correspondence of low- energy-to-high-energy displacement damage effects in electronic materials (e.g., GaAs and GaN) and (2) Understanding single event and stochastic effects in component circuitry (e.g., transistors).
- **Combined Environments:** Most test and qualification activities assess component and sub-system response to individual, independent radiation environments (e.g., EMP, gamma-rays, neutrons, or x-rays). Treatment of combined environments can be a challenge if one needs to go

beyond merely noting that, for instance, the total dose to a component is consistent with the addition of all environments. Key research challenges include (1) Understanding effects of EM coupling through points of entry and shielding effectiveness under mechanically dynamic conditions and (2) Developing diagnostics for combined environments.

- **Modeling and simulation:** High fidelity, three-dimensional simulation of radiation environments and effects requires highly coupled, multi-physics, multi-scale models that range from an atomistic description of radiation interaction with matter to full system circuit and material response. Moreover, we must rigorously validate the models with experimental data. Key research challenges include (1) Making advances in air chemistry, hybrid kinetic/fluid plasma models; (2) Coupled radiation/EM/Plasma environment modeling; and (3) Inventing advanced algorithms to overcome runtime issues related to problem scale sizes.

REHEDS2:

High Energy Density Sciences (HEDS)

The HED science effort focuses on the creation, understanding, and application of matter at extreme energy densities, including the study of Inertial Confinement Fusion. We are soliciting proposals in the following topical areas to address a number of applied and computational challenges that have been identified.

- **Novel Fusion Platforms for > 100 MJ:** Today our major efforts are focused upon establishing the physics basis and determining the pulsed-power requirements for scaling ICF target concepts such as magnetic direct drive (MDD) from Z to a future facility where multi-MJ and high fusion yield is possible. A key research challenge with this work lies with (1) Extending the capabilities of magneto-radiation-hydrodynamic codes to model that evolution over a broad range of plasma densities, thereby demonstrating control of the implosions across a range of convergence requirements and routinely measuring and modeling the 3D nature of the implosions and (2) Developing diagnostics and advanced data analysis methods to quantify inferred performance metrics and assess 3D character of implosions.
- **Material & Opacity Science:** Material science challenges include improving measurement capabilities for key properties such as the temperature and phase of materials under dynamic compression. Another challenge is the measurement and modeling of time-dependent phase-transition phenomena and investigating the often-complex structure-property-performance relationships associated with materials that are aging or are newly manufactured with either traditional or advanced manufacturing techniques. These studies often include investigation of material opacities at high temperature and density. Key science challenges in this area include: (1) Measurement capabilities (*e.g.*, temperature and phase); (2) Time dependent kinetics; (3) Higher throughput and accuracy for opacity platforms; and (4) Measured versus calculated opacity.
- **Cold and Warm X-ray radiation environment:** HED plasmas provide some of the brightest cold and warm x-ray and fast neutron environments for weapon survivability testing. Z-pinch implosions on Z currently form the brightest source of cold x-rays (1-5 keV) and, together with NIF, warm x-rays (5-30 keV) in a laboratory setting. Here our applied science challenges include (1) Advancing our capabilities with making precision measurements of the radiation environment.

REHEDS3:

Electrical & Electromagnetic Science (EES)

Electrical and Electromagnetic Science proposals are solicited in the following topical areas to help advance our understanding of key electrical phenomena relevant to the nuclear deterrence and broader national security missions. That portfolio covers electrical circuit and device response to radiation and electromagnetic environments, as well as EM environments in both physical and computational simulation domains.

- **Electromagnetic environments and effects:** National security systems rely heavily upon electronics to ensure mission success. All systems must operate in electromagnetic radiation environments that may have deleterious effects on the performance of critical electronics. Key research challenges in this area include (1) Improving the performance of high-fidelity simulations of high-Q cavity coupling at fields above 30 GHz and in combined mechanical vibration and EMR environments and (2) Exploration of utility and approaches to artificial intelligence and related data analytics for the analysis of fused test and simulation data.

Future high-performance electrical generation systems: Technologies are desired to improve system performance through incorporating advanced control design capabilities that enable power electronic systems to operate to extremes, including near stability margins or in nonlinear regimes. Key research challenges in this area include (1) Creation of topologies and functions that can change how energy is transferred and converted in power electronic and power systems, (2) Enabling design of high-power-density electrical conversion circuits ensuring long-term reliability without electrical breakdown or electromagnetic coupling issues and with optimized frequency response while operating in Earth and near-Earth electrical/plasma environments and (3) Enabling multiphysics/multifunction-based designs that account for interactions with other systems.

REHEDS4:

Pulsed Power Science & Technologies

Pulsed power science and technology underpins much of the work in this IA, and, as such, any developments in pulsed power benefitting the operation of Sandia facilities can have an enormous impact on what we do. To advance this science and technology, proposals are solicited which will improve the understanding of key research challenges like (1) High voltage breakdown, (2) Power flow and plasma formation, (3) Predictive maintenance and improved reliability, (4) Improved containment concepts.