University of California Office of President
Request for Proposals
Artificial Intelligence Science at Scale

University of California Research & Innovation (UCR&I),
University of California National Laboratories (UCNL),
University of California Office of President (UCOP)

November 4, 2024

Timeline	Dates
Call for Workshop and Interest	September, 2024
AI Workshop at UC Riverside	October 16, 2024
Issue Request for Proposal	November 4, 2024
Pre-Proposal Due	December 20, 2024
Notification for Final Proposal	January 17, 2025
Final Proposal Due	March 18, 2025
Notification of Winning Proposals	April 15, 2025

Request for Proposals

Funding Opportunity Program Description

Introduction and Goals

The University of California (UC) system, in partnership with the UC-managed National Nuclear Security Administration (NNSA) national laboratories, Los Alamos and Lawrence Livermore National Laboratories, (LANL and LLNL, respectively), is seeking proposals from University of California researchers for collaborative projects that advance the frontiers of Artificial Intelligence (AI) and Machine Learning (ML) science at scale.

Our central goal is to bring together the intellectual power of the UC system, including 10 leading public research universities and 3 national laboratories, and develop scientific AI projects that benefit from computational scale while also harnessing the power of interdisciplinary AI and science and engineering research and expertise. These efforts – scaled up by a focus on both large AI models and cross-cutting teams – should operate seamlessly across multiple campuses while deeply integrating with national laboratories. These efforts must address critical challenges in national security, scientific discovery, and technological innovation – and must do so at scale.

Successful proposals are expected to clearly define an end-to-end solution that drives the proposal while developing and incorporating new AI techniques. In addition, proposals are expected to be synergistic with existing AI programs at LANL and/or LLNL.

By building robust, interdisciplinary teams, we aim to leverage novel AI techniques, computational resources, and domain expertise to develop scalable solutions that significantly advance key application areas, including Multiphysics Applications, Biological Systems, and Materials Discovery.

Teams should focus both on developing exciting new AI capabilities for science and on driving forward a single specific Technical Focus Area.

Technical Focus Areas

Successful proposals will deliver a cohesive AI ecosystem that drives forward a single, focused application area. Projects should develop a unified interdisciplinary team with AI researchers and subject matter experts that jointly create a scientific AI system for the specific application built around novel AI contributions. Ideally, the proposed AI methods transcend the subject matter area and generalize to a wider range of problems; however, the work and vision should be built specifically for only one of the application areas below.

1. **Multiphysics Applications**

Objective: Develop AI-driven solutions to improve multi-physics simulation capabilities guided by a well-defined end-to-end science driver that involves multiple spatial and temporal scales. Example problem domains include natural hazards, complex engineered systems, renewable and sustainable energy, fusion energy, fluid flow and transport, astrophysics and cosmology, climate models including catastrophic events, carbon capture, and multiscale CFD.

Key AI Challenges:

- How can we develop and utilize inverse problems to design systems with desired properties incorporating physical and geometric constraints and target tolerances/uncertainties, or accelerate the systematic exploration of a multidimensional design space?
- How can AI algorithms that explicitly use physics knowledge during the training process to improve algorithm performance?
- Can we develop AI methods to predict rare/extreme/catastrophic events with quantifiable uncertainties?
- How do we develop comprehensive methods & tools for preparing diverse data for use in training and/or inference?

Approaches of Interest:

- Integrative approaches that strive to iteratively improve the accuracy of predicted quantities for the science driver via successive improvements in AI methods & tools
- Collaborations with, potentially external, partners to facilitate the use of large diverse datasets essential for AI training and/or model validation for the science driver
- Vision transformers and other methods for representing spatial-temporal data
- diffusion models
- Modifications to transformers and other modern architectures to incorporate physics constraints
- Methods for uncertainty quantification

2. **Biological Systems**

Objective: Create foundation models across scales that predict biological functions and evolutionary dynamics within complex ecosystems and build new molecules using AI-driven design and synthesis techniques.

Key Challenges:

- How can LLMs be used to predict nucleic acid and protein sequence functions or model the evolution of organisms in dynamic ecological systems?
- Can AI models integrate vast amounts of genomic data to predict biological behaviors at scale?
- What AI techniques can be developed or adapted to design and synthesize new molecules, ensuring they possess desired functions or properties?

- How can empirical data from experimental systems be effectively used to refine and validate AI-driven molecular design?

Approaches of Interest:

- Collaboration with partners possessing large biological datasets, such as genotype-phenotype correlations or experimental evolution data, or clinical evidence for validation.
- Development of automated laboratories that generate data for deep learning models in biological contexts.
- Development of advanced molecular representations for AI model training (can include small molecules, proteins, etc.), to improve the accuracy and applicability of AI models in predicting biological functions and properties.
- New or adapted AI/foundation model architectures that exploit data representations of molecular data, enabling the creation of more sophisticated and precise AI models for biological systems.
- AI models or Digital Twins that integrate first-principles molecular predictions and new AI models (LLMs integrated with above new models, generative molecular tools, etc.) to produce highly scalable computational molecular generators, disease and intervention predictions.
- Associated synthesis pathways and chemical precursors, to be predicted by the integrated systems, enabling a comprehensive approach to molecular design and synthesis.
- Coupling to edge systems, or automated chemistry systems or cloud labs, that can test hypothetical molecules and pathways, ensuring that AI predictions can be practically tested and validated in real-time.
- Design of experiments or measurements to confirm successful synthesis, providing empirical validation of AI-generated molecular designs.
- Closed-loop operation that uses empirical observations to inform selection of the next best hypothetical molecule, facilitating continuous improvement in molecular design processes based on real-world feedback.

3. Materials Discovery

Objective: Apply AI/ML techniques to one or more of the stages of the materials discovery pipeline, from predicting structure and properties to inverse design, experimental synthesis, manufacturing, and deployment. Of particular interest are the prediction of properties such as mechanical response for high entropy alloys or properties relevant for materials for clean tech or electrochemistry, to name a few examples. Teams should focus on deep integration of AI for a particular material or class of materials with the end-to-end pipeline in mind, while not necessarily focusing on all parts of the pipeline.

Key Challenges:

- Can AI models be developed to predict material properties at multiple scales (from molecular to continuum) and optimize material design accordingly?

- How can multimodal data from experiments and simulations be leveraged to improve material design processes?
- How to integrate existing scientific literature and use it for analysis and prediction?
- How to explain and reason about material design and synthesis pathways?
- How to build AI models using sparse data?

Approaches of Interest:

- AI models coupled to physics models that "invert" the material design to yield desired properties, facilitating targeted material development.
- AI models that bridge scales from molecular to meso, to continuum scale, improving the accuracy of property estimation across various levels of material structure.
- AI models that explain how properties of materials are coupled across scales.
- Multitask models that also develop production pathways and testing methods, ensuring that designed materials can be practically produced and tested. Design of experiments and material synthesis pathways that are tightly integrated with AI prediction tools.
- Development of foundation models or tuning of Large Language Models to predict, analyze, and generate materials and synthesis pathways.
- AI models that adapt to sparse data, or more generally improve quality of raw data.

Elements of a Coherent AI Ecosystem

Proposals should not only aim to advance specific application area(s) but also contribute to strengthening the broader AI ecosystem that establishes partnerships spanning academia and national laboratories. For example, the proposal could emphasize the importance of a holistic approach where work on applications is tightly integrated with and enhances three foundational elements: Data, Models, and Compute.

1. **Data:**
    - **Integration with Applications:** Proposals should focus on creating or leveraging innovative data methods that enhance the quality, availability, and usability of data across the AI ecosystem. This includes the development of new data representations, tokenization strategies, and data pipelines that facilitate the flow of information between experimental, simulated, and real-world data sources.
    - **Strengthening the Ecosystem:** By advancing data methodologies within your application area, your work should help establish robust data practices that benefit other areas of research. For instance, methods developed for handling large, multimodal datasets in one application should be applicable to other domains, thereby improving data consistency and accessibility across the ecosystem.
2. **Models:**

- **Integration with Applications:** Proposals should aim to develop or adapt AI models that are not only suitable for the specific application but also contribute to broader modeling frameworks. This includes creating scalable architectures, improving training processes, and ensuring model robustness and validity.
- **Strengthening the Ecosystem:** Work on application-specific models should lead to advances that can be generalized or transferred to other contexts, thus enriching the overall modeling capability within the AI ecosystem. For example, techniques developed to ensure model accuracy and scalability in a biological application might be adapted to improve model performance in materials science or multi-physics simulations.

3. **Compute:**
    - **Integration with Applications:** Proposals should consider the computational demands of AI at scale, proposing methods that optimize the use of national laboratory assets, cloud resources, and emerging hardware. This includes addressing challenges related to strong and weak scaling, parallelism, and computational efficiency.
    - **Strengthening the Ecosystem:** By developing compute strategies that address the specific needs of your application, your work should also contribute to the optimization of computational resources across the AI ecosystem. This could involve creating new algorithms or tools that improve the efficiency of AI workloads, which can then be used in other research areas to enhance overall computational capabilities.

In designing your project, consider how work in one application area (e.g., Multiphysics Applications, Biological Systems, or Materials Discovery) can simultaneously contribute to and benefit from advances in data, models, and compute. A successful proposal will demonstrate a clear strategy for closing the loop between these elements, ensuring that progress in one area supports and is supported by the others, ultimately leading to a more cohesive and powerful AI ecosystem.

Solutions for the technical areas must build novel AI contributions to the scientific AI ecosystem. Application of existing or traditional ML methods to application areas will not be sufficient. Transformational methods might include, but are certainly not limited to:

- AI surrogates with uncertainty quantification (UQ) and accelerators to optimize predictive accuracy and scalability of numerical tools.
- AI models trained with advanced data representations, new multimodal agents to integrate empirical and numerical data, and multitask models.
- Data centric AI tools to improve quality of raw data from various science domains, such as data augmentation and synthetic data generation
- AI reasoning systems for reliable multiscale and multidomain predictions, and multiscale physics models combining first-principles and AI predictions.

- Experimental design with deep reinforcement learning, AI predictions connected to real-world facilities for validation, and closed design loops exploiting empirical data for continuous AI model refinement.
- Mitigation of hallucinations from large AI models, expanded explainability of performance, enhanced reliability in the decision-making process (including quantifying uncertainty)
- Theoretical contributions in all of the above.

Award Details and Requirements:

Award Term and Funding Request:

One award per each of the three technical focus areas: Multiphysics Applications, Biological Systems, or Materials Discovery. The proposals may request three years of support. The funding request for the technical focus area proposals is expected to be ~$6 million (including indirect costs) for a three-year award term.

Each team must comprise participation of a minimum of three, preferably four, UC campuses, plus participation from one or both of the UC-managed NNSA national laboratories (Los Alamos and Lawrence Livermore National Laboratories).

Total annual project costs in excess of the allowable maximum may be covered by other sources of support or contributions (see "NNSA National Laboratory contribution" below).

Total budgets must be well-justified in relation to the proposed activities and potential impact of the proposal. Funding should prioritize research and training support for UC students and postdoctoral scholars, particularly support for activities that advance graduate students to degree. Proposed budgets should seek to efficiently use resources to maximize research outcomes and minimize administrative costs. An itemized budget and justification for each collaborating institution is required in the full proposal.

Allowable and Non-Allowable Costs:
The full application instructions will include instructions on allowable and non-allowable costs. Both UC campuses and the NNSA and DOE Office of Science national laboratories may charge their approved indirect cost rate (MTDC basis) to the award. As general guidance, please be aware that funds provided by this award may not cover any classified research activities, patient care costs, clinical trials, patent execution costs, fundraising costs, equipment maintenance, or subawards to non-UC-affiliated entities. Equipment purchases by the national laboratories or for national user facilities are not allowed. Equipment purchases by UC campuses may be requested if a compelling justification is provided, and use of and access to the equipment is made available across the UC system. Equipment must permanently reside at a UC campus location and may not be purchased for permanent installation at a non-UC location.

NNSA National Laboratory Contributions:
Recognizing that the NNSA national laboratories have unique resources, facilities, expertise, data, and other research infrastructure that will ensure both mutual benefit and successful outcomes, proposals are expected to identify specific contributions and facility access that each participating national laboratory will make to the collaborative endeavor. Contributions may include space, equipment or facilities use, data, or expertise that may be covered by other sources of support or directly relevant activities at the laboratory. The participating national laboratories describe the specific laboratory contributions to the proposed research on the "List of Facility and Other Resources needed to support this proposal" tab of the full proposal application.

LLNL/LANL Participant Expectations and Funding:

In the event of a successful award, the LLNL/LANL Co-Investigators and any other laboratory partners will work with that UC faculty member for the duration of the award (up to 3 years).

It is the NNSA national laboratory participants' responsibility to work closely with their programmatic leadership to determine appropriate funding, obtain permission from the laboratory leadership before the full proposal submission, and it is anticipated that these activities will be part of the laboratory employees' roles and responsibilities and regular job activities, which usually include activities such as research and development, partnership and collaboration, pipeline development and workforce recruitment, among others.

In addition, laboratory PI's programmatic leadership will need to make accommodations for their staff members to work with UC faculty on proposal development and associated pre- and post-award activities.

Lawrence Berkeley National Laboratory (LBNL) Participant Expectations and Funding:

LBNL is a DOE Office of Science national laboratory and part of the UC system. For this proposal process, LBNL staff is regarded as a UC institution, similar to a UC campus. LBNL staff are encouraged to participate as co-investigators of a proposal team. Request for funding is anticipated in modest amounts, but in any case, no more than 0.05 FTE per year.

LBNL's Strategic Partnership Projects office must review the proposed budget and commitments included in the proposal, and the institutional signing official must submit an approval form with the application. In addition, each proposal must include a letter affirming the specific commitments requested in the project budget that laboratory will make if the proposal is awarded, and this letter must be signed by the designated laboratory official.

Commitment to Sustain UC – National Laboratory Collaborations:

Collaborations should demonstrate a commitment to deep, sustained engagement between UC and the national laboratories that will extend beyond the award period. The proposal should include a specific plan for periodic meetings of the faculty, scientists, postdoctoral scholars, and graduate students from the multiple institutions that comprise the proposal team.

Eligible Institutions and Systemwide Collaboration:

The applicant institution submitting the proposal on behalf of the collaboration must be one of the 10 UC campuses (Berkeley, Davis, Irvine, Los Angeles, Merced, Riverside, San Diego, San Francisco, Santa Barbara, or Santa Cruz). In addition to the applicant institution, the proposal team requires a minimum of two, preferably three *additional* UC campuses, plus participation from one or both of the NNSA National Laboratories (Los Alamos and Lawrence Livermore National Laboratories). LBNL participation is also encouraged.

For the pre-proposal, the proposal team membership should comprise of only UC PI, co-PI, and co-investigators from each campus, and co-investigators from LBNL. The pre-proposals should be aligned with the goals of the national laboratories based on the workshop and the RFP.

Note: Each collaborating UC campus or other eligible UC research location will be designated as a "sub-contractor" to the applicant UC campus. Each collaborating UC-managed national laboratory will directly contract with the UC Office of the President and complete a separate prime budget and institutional approval form from designated national laboratory offices. *UC National Laboratory Fees Research Program Collaborative Research and Training Awards RFP – Award Year 2025 v. April 2, 2024, p.* 3

Exclusions:

- Research partners from outside the UC system may not participate in this proposed collaboration.
- The UC Office of the President and its personnel may not participate in any proposal, and funding may not support activities at the UC Office of the President.

Eligible Principal Investigators:

The proposal must be submitted by a UC faculty member who holds Principal Investigator (PI) status at the applicant UC campus. The Applicant PI is the designated Principal Investigator for the award. Each collaborating institution (UC campus) may also identify Co-Principal Investigator(s). A Co-Principal Investigator (Co-PI) is a person who shares the responsibility and authority of a research project's leadership and direction with the PI. All Co-PIs must also hold PI status at their respective institutions. Each proposal will consist of one PI, and the number of the co-PIs depends on the proposed team structure and roles and responsibilities. For guidelines on UC PI status, contact your campus Office of Sponsored Research or refer to Section 1-530 of the UC Contracts and Grants Manual.

Individuals with joint or shared appointments at multiple locations must apply through the location of their primary appointment. For individuals with multi-location appointments (MLAs), their primary appointment is typically the location through which they receive their salary and benefits.

Individuals with joint or shared appointments at a UC campus and a national laboratory are encouraged to consult with their campus Office of Research and the National Laboratory contact listed in the RFP prior to submitting their proposal.

Proposals may include additional key personnel at any of the eligible collaborating institutions if they contribute substantively to the proposed research. Additional key personnel at each site must be designated as Co-Investigators (Co-Is), named trainees, or other allowable roles consistent with their status and contributions. Proposals that involve faculty, students, postdocs and other trainees historically underrepresented in the identified fields are encouraged.

National laboratory staff members participating in the proposals are Co-Is.

Exclusions:

- A UC campus faculty can participate as a PI or Co-PI on only one proposal, but can participate as Co-I on multiple proposals.
- Academic personnel whose primary role is in university-wide, campus, or school administration above the level of Dean, or individuals whose primary role is national laboratory leadership or administration, may not serve as PIs, Co-PIs, or Co-Is on the proposal.

Award Requirements:

- The full proposal submission must be a joint technical proposal with LANL and/or LLNL technical staff member(s). National laboratory staff will serve as Co-Investigators on the team.
- Members of each UC research group are highly encouraged to engage research at either LLNL or LANL during the funding period.
    - Access to NNSA National Laboratory resources—including institutional computing resources—and facilities requires an external collaborator to have a vetted relationship and approvals in place with the National Laboratory. In order to gain system or site access, a UC collaborator will need to provide the National Laboratory with information required to secure necessary approvals. If a UC collaborator is a foreign national, then additional approvals will be required for system or site access.

Proposal and Review Process and Timelines:

The proposal process will include two phases, a pre-proposal phase and a full proposal phase.

- The pre-proposals (proposal template in Appendix A) will include the intended team members and a short (3 pages) description of the team's technical focus and approach.
- The pre-proposals will be evaluated by a UC Screening committee consisting of senior UC/National Lab leaders and subject matter experts. The review criteria will be focused on the technical merit of the proposal.
- The Screening Committee will invite two to three teams per technical focus area to submit full proposals.
  - Submission instructions will be sent to the teams invited to submit full proposals.
  - Full proposal template is in Appendix B.
- The Screening Committee will recommend the recipients for the award to the Executive Steering Committee. The Executive Steering Committee will be responsible for making the final selection.

Pre-proposal Submissions

Please submit the pre-proposals by **December 20, 2024**. The required elements for the pre-proposal are described in Appendix A.

Please submit pre-proposal to: universitycollaborations@lanl.gov

Pre-proposal Reviews

The Screening and Selection Committees will review the pre-proposals and notified the teams to submit full proposals by **January 17, 2025**.

Final Proposal Submissions

Please submit the final proposals by **March 18, 2025**. The required elements for the full proposal are described in Appendix B.

Notification of Award:

The winning recipient of the award will be announced by **April 15, 2025.**

Upon announcement, UCOP will be in contact with the winning team to discuss mechanism to commence funding distribution.

UCOP reserves the right to reject a proposal without review including for the following reasons:

- The proposal is clearly nonresponsive to the objectives and/or provisions of the call for proposal.
- The proposal does not meet the requirements for proposal format, content, and organization as specified in the stated guidelines.
- The proposal is not submitted by the submission due date/time.

Review Process during Award Cycle:

The award recipients are requested to report back to the UC community on an agreeable schedule during the 3-year award period. Award renewal will be considered if there are no changes in the following items:

- The fundamental technical scope as proposed.
- The team members remain in good standing at the UC.

Award Selection Process and Criteria:

Screening Committee:
The responsibility of the Screening Committee is to

- Review the pre-proposal and down select the pre-proposals to the top two to three proposals and invite those teams to submit full proposals.
- Review the final proposals and recommend the winning team to receive funding and commence research activities.

The Screening Committee will be selected by the Executive Steering Committee consisting of:

- Rodolfo Torres, Vice Chancellor of Research, UC Riverside
- Pramod Khargonekar, Vice Chancellor of Research, UC Irvine
- Katherine Yelick, Vice Chancellor of Research, UC Berkeley
- Theresa Maldonado, VP, Research and Innovation, UCOP
- June Yu, VP, National Laboratories, UCOP
- Duncan McBranch, Senior Director, Partnerships and Pipelines Office, Los Alamos National Laboratory

Review Criteria:
SCIENTIFIC AND/OR TECHNICAL MERIT OF THE PROJECT (50%)

- What is the scientific innovation of the proposed research?
- How would the proposal leverage novel AI techniques, computational resources, and domain expertise to develop scalable solutions that significantly advance key application areas, for example, a new foundation model?
- How well did the proposal develop scientific AI systems that benefit from computational scale?
- How well did the proposal harness the power of interdisciplinary AI and science expertise?
- What is the likelihood of realistically achieving high impact results?
    - Are the conceptual framework, methods, and analyses well justified, adequately developed, and likely to lead to scientifically valid conclusions?
    - Does the applicant recognize significant potential problems and consider alternative strategies?
    - Does the proposal significantly advance the state of the art for the science driver?
- What is the long-term sustainability of the research beyond the current proposal. What is the vision beyond the current funding cycle?
- How can this proposal contribute to the establishment of the foundation for future funding opportunities, such as the possible Frontiers of Artificial Intelligence for Science, Security, and Technology (FASST) initiative?

TEAM COMPOSITION, QUALIFICATIONS, AND INTEGRATION; AND ADEQUACY OF PROPOSED RESOURCES (25%)

- How well qualified is the research team to carry out the proposed research?
- Are there clear roles and responsibilities defined in the team to ensure communication and integration
- Does the proposal clarify how the individual activities lead to advances in the state of the art for the science driver through their integration?
- Are the proposed budget and staffing levels adequate to carry out the proposed research?
- Is the budget reasonable and appropriate for the scope?
- In addition to funding, what resources would be needed to ensure achieving technical objectives and milestones outlined in the proposal? Consider the resource requirements to achieve objectives and how likely can the proposal acquire the stated needs.
    - What are the computational resources needed?
    - What are the experimental resources needed?
    - What is your UC and national laboratory faculty-staff engagement model?

UC/NATIONAL LABS ENGAGEMENT MODEL, INCLUDING UTILIZATION OF LABORATORY AND UC RESOURCES, SUCH AS DATA, COMPUTATIONAL AND EXPERIMENTAL CAPABILITIES, AND UC/LAB FACULTY-STAFF ENGAGEMENTS. (25%)

- Alignment between UC and the national labs on research interests and technical focus area to which the application is submitted.
    - How would the UC faculty and research group engage with LANL and LLNL?
- How would the proposal evolve to a longer-term pipeline for funneling UC students and post-docs to the national laboratories?
- Does the proposed work take advantage of unique facilities and capabilities at the Universities, LLNL, and LANL?
- Is the Data Management Plan suitable for the proposed research?
    - To what extent does it support the validation of research results?
    - To what extent will research products, including data, be made available and reusable to advance the field of research?
- How would you manage, share, access, or curate data?

Award Sponsors:

<u>University of California Research and Innovation (UCR&I) and National Laboratory (UCNL) Offices, University of California Office of President (UCOP)</u>

UCR&I and UCNL are partners in providing resources and support to foster a strong UC-National Laboratories research partnership and collaborations. UCNL plays a central role in providing leadership, management, and stewardship of the three UC affiliated national laboratories while informing The Regents and the UC President of National Laboratory compliance and performance issues.

Laboratory Contacts and Resources

UC faculty with questions about the process or approach to forming collaborations with the national laboratories in the targeted area are encouraged to contact the national laboratory Points of Contact identified below and consult the suggested resources:

Lawrence Livermore National Laboratory
Eric Schwegler, PhD – Director, Academic Engagement Office & Science Education, schwegler1@llnl.gov

Los Alamos National Laboratory
Heather H. Erpenbeck, PhD – University Collaborations Office Leader, hawk14@lanl.gov

For further technical information, please consult:

- LANL:
    - Artificial Intelligence
    - AI Signature Institutional Commitment
- LLNL:
    - Data Science Institute
    - AI Innovation Incubator

For the recorded video link of the plenary session of the AI Science at Scale Workshop at UC Riverside on October 16, 2024, please go to:

Link to the plenary presentations at the AI Science at Scale Workshop at UC Riverside

AI Foundations:
https://drive.google.com/drive/folders/1HzeO2TQvnss9zjqf1__92FlyY-eCWj3k?usp=sharing

Materials Science:
https://drive.google.com/drive/folders/1jX8zc76hiWrh5EJRn031gOdcB1AcXIqX?usp=sharing

Biology:
https://drive.google.com/drive/folders/1uK-L4HtdiPkrChW9VfIHDDgcs9VGortq?usp=sharing

Multiphysics:
https://drive.google.com/drive/folders/1OxbArQdNZudppKjwlhDwHeTBm63LwU6I?usp=sharing

Link to the plenary talks at the workshop

https://urldefense.com/v3/__https://drive.google.com/drive/u/1/folders/1w91sSsL75AGLdWnedN7GYJgBWVk276Gq__;!!Bt8fGhp8LhKGRg!HFJ2l6vdyxqMmacVVSt5vCawq5xaEAO8kFqYRjc6vNYtTI797jcq4V2y1LLuAznrPgLMYjnX9EeMSU9dOe4w$

Link to the slides for the plenary presentations:
https://drive.google.com/drive/folders/1GhxnVidUYZuADZoHIQeKhDzL3J-BahoM?usp=sharing

Appendix A: Pre-proposal Template

- Please submit pre-proposal to: universitycollaborations@lanl.gov

Summary Table

Proposal Name	
Primary Technical Focus Area	
Short (1 to 2 line) Description	
Name/Department of UC PI, co-Pi, and co-investigators and contact info	
PI, co-Pi, and co-investigators' affiliated UC campus	

Proposal Description (3 pages)

A description of the problem, why this research and development is needed and how it relates to the technical focus area, your proposed solution and approach, existing research (if any) you are building upon, and measure of success.

In drafting the pre-proposal, please focus on the technical merit of the proposal. Review Committee will consider evaluation criteria, including:

- What is the scientific innovation of the proposed research?
- How would the proposal leverage novel AI techniques, computational resources, and domain expertise to develop scalable solutions that significantly advance key application areas, for example, a new foundation model?
- How well did the proposal develop scientific AI systems that benefit from computational scale
- How well did the proposal harness the power of interdisciplinary AI and science expertise
- What is the likelihood of realistically achieving high impact results?
    - Are the conceptual framework, methods, and analyses well justified, adequately developed, and likely to lead to scientifically valid conclusions?
    - Does the applicant recognize significant potential problems and consider alternative strategies?
    - Does the proposal significantly advance the state of the art for the science driver?
- What is the long-term sustainability of the research beyond the current proposal. What is the vision beyond the current funding cycle?
- How can this proposal contribute to the establishment of the foundation for future funding opportunities, such as the possible FASST AI research initiative?

Appendix B: Final Proposal Template

- Submission link will be provided to the teams invited to submit full proposals

Proposal Cover Page

Each proposal shall include a *Proposal Cover Page* with a Summary Table (description below).

Summary Table

Proposal Name	
Short (1 to 2 line) Description	
Name/Department of UC Principal Investigators	
PI, Co-PI, and Co-investigator's address	
PI, Co-PI, and Co-investigator's contact information	
PI, Co-PI, and Co-investigator's affiliated UC campus	
Name/Org of LANL/LLNL collaborator(s)	
Cost/year including	
● Cost for university per year	
● Other, e.g., travel, equipment (with justification), etc. (describe)	
Total cost/year (must be under $1,700K/yr for an aggregate of $5M/3 years)	
Estimated effort for each Lab collaborators. (Note that funding for Lab collaborators is not included in award and Lab collaborators need to obtain Lab program approval prior to proposal submission.)	

Proposal Summary (Abstract):

Please include a Proposal Summary suitable for release through a publicly accessible archive should the proposal be selected. The Proposal Summary should be concise, should not exceed 4,000 characters in length, and should not contain any special characters, graphics, or formatting (use text only).

Description of your proposal (<10 pages, excluding references)

A description of the problem, why this research and development is needed and how it relates to AI and the technical focus area, your proposed solution and approach, existing research (if any) you are building upon, and measure of success. How would the proposal address the review criteria listed in the RFP?

How does the University/Lab collaborative project support one or more of the following outcomes?

- Innovation in methodologies or processes, contributing toward basic science understanding, or providing independent perspective on existing methodologies or scientific understanding with potential paths forward.
- Product (e.g., data, laboratory validated technology, implementable methodology)
- Student's and Post-doc's development

What is the plan to forming a truly collaborative, trusting University/Lab relationship? What is the expected method and level of university engagement?

Expected Milestones and Deliverables (interim and final)

Please provide interim (at least yearly) milestones and deliverables, as well as final deliverables.

Data Management Plan (1 page)

What is the data management needs and strategy, including data management and access from both the Universities and Laboratories?

Budget Proposal (for the duration of the project)

Proposers need to include budget figures for all years of the proposed project and summarize the budget proposal in the Summary Table. The proposal needs to justify the proposed budget, including the overhead rates (including indirect and benefits) for UC, LBNL, and LLNL/LANL.

Budget proposal should include:

- UC faculty, researchers, and LBNL staff's salary covered by this proposal.
    - Funds requested for fringe benefits must be calculated as the product of the requested salary and, if present, the negotiated fringe benefit rate contained in an institution's negotiated indirect cost rate agreement.
    - Funds requested for indirect costs must be calculated using the correct indirect cost base and the negotiated indirect cost rate.
- Students' salaries (including both undergraduate and graduate students).
- Postdocs' salaries.
- Administrative support staff's salaries
- Equipment and supplies, including laboratory and computational needs.
    - Equipment is designated as an item of property that has an acquisition cost of $5,000 or more and an expected service life of more than one year

    - Enter total funds requested for materials and supplies
    - Enter total funds requested for Computer Services. The cost of computer services, including computer-based retrieval of scientific, technical and education information may be requested
- Travel, including conferences and Lab visits.
- Publication costs
    - Enter the total publication funds requested. The proposal budget may request funds for the costs of documenting, preparing, publishing or otherwise making available to others the findings and products of the work conducted under the award
- LLNL/LANL Participant Expectations and Funding
    - Please refer to details in the RFP.

List of Facility and Other Resources needed to support this proposal

What are the resource needs from the Laboratories to achieve the technical objectives? Please work with your laboratory team members to identify the needed resources and how to access them. For more questions, you can refer to the Laboratory Points of Contacts listed in the RFP.

Proposal Team: (please include UC faculty and Lab staff's bio or curriculum vitae (CV), not included in page count limit)

Team Composition (1 page)

A Collaboration Plan where the roles and responsibilities of the PI and team members are clearly explained. For example, some of the possible roles and responsibilities: team integration, data officer, project manager, etc.