NATIONAL SCIENCE FOUNDATION
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ALEXANDRIA, VIRGINIA 22314

NSF 21-080

Dear Colleague Letter: Advancing Discovery with AI-Powered Tools (ADAPT) in the Mathematical and Physical Sciences

May 5, 2021

Dear Colleagues:

The tools and techniques of Artificial Intelligence (AI) are transforming discovery in the disciplines traditionally supported within the Directorate for Mathematical and Physical Sciences (MPS). This transformation has been enabled by academic and private sector developments leading to increased computing power, improvements of AI algorithms, and the availability of large and complex data sets. MPS researchers tackle problems that can drive advances in the foundations of AI, and synergies between research frontiers in AI and in MPS can stimulate further potentially transformative progress. Sustained and meaningful collaborations between AI and the MPS disciplines will transform scientific discovery and deliver broader societal benefits.

This Dear Colleague Letter (DCL) welcomes proposals for the development or new application of AI-inspired tools and techniques, with opportunities in, but not limited to, four focus areas: (i) modeling and simulation, (ii) data and model analytics, (iii) concept discovery, and (iv) physical systems/experimentation. Successful proposals will advance MPS science goals and at least one of the following focus areas:

- AI for Modeling and Simulation

  The increasing use of high-dimensional data demands new approaches to modeling and simulation. Proposals can address current limitations in critical and complex problem-solving methods. Areas of research may include new mathematical, statistical, data-driven and complex system modeling, stochastic and numerical simulations, experiment design, data assimilation, and validation. Proposals that advance pattern recognition simulation, and comparison or optimization of pathways towards targeted endpoints are also encouraged.

- AI for Data and Model Analytics

Extracting science from data is tied to the processing methods. Proposals are encouraged for advances in algorithms, improvement of feature extraction, image analysis, robust classification and clustering, and interpretability. Areas of research may include AI algorithms that respect physical laws or mathematical constraints, and that streamline and prioritize data collection, work with heterogeneous data, and human-machine interfaces. Additionally, work that advances foundational topics such as supervised and unsupervised learning, optimization, and generative adversarial networks is also encouraged.

- AI for Concept Discovery

  Proposals can use domain science challenges to inspire cutting-edge advances in machine learning to accelerate discovery of new concepts and better understand phenomena in the physical sciences. For example, this may be achieved by interpreting AI models to provide clues to the structure of a theory or by using AI models to link patterns to an understandable interplay of physical properties. Concept discovery may be applied in the analysis of large or small data sets.

- AI in Physical Systems and Experimentation

  The MPS experimental and observational sciences rely on data collection at both large and small scales. Some programs depend on facilities that produce large volumes of data that may depend on complex physical configurations, workflows, and environmental conditions. Other programs are working towards advances in data collection to expand capacity for pattern recognition. Proposals may address AI-enabled tools and new AI applications that transform experimental design in both large and small data settings. Proposals may also address the challenges of real-time decision and experiment control, workflow optimization, and the hardware implementation of AI algorithms in embedded or robotic systems.

The Directorate for Mathematical and Physical Sciences welcomes proposals for large and small projects addressing complex problems at the frontiers of AI, that align with current divisional interests. Projects that establish new collaborations between academia and industry, broaden participation, train an AI-aware workforce, or promote interdisciplinary activities are especially encouraged. Proposals that promote collaboration among MPS domain sciences and researchers with AI expertise will be prioritized. Proposals should be submitted using the mechanisms described below.

1. Supplemental funding requests:
   a. Supplemental funding requests to existing NSF awards that extend existing AI activities or expand the scope of the project to include the development of new AI techniques and applications. These additional activities could include new

       collaborations that strengthen a team's AI expertise.

    b. GOALI (Grant Opportunities for Academic Liaison with Industry) is a "type of proposal that seeks to stimulate collaboration between academic research institutions and industry." To that end, we encourage submission of GOALI supplemental funding requests to existing MPS awards that address shared AI interests by academic researchers and industrial partners, and which foster meaningful collaboration to both advance MPS science and AI.

    c. INTERN (Non-Academic Research Internships for Graduate Students) supplements provide up to six additional months of support for graduate students to gain knowledge, skills and experiences that will augment their preparation for a successful long-term career through an internship in a non-academic setting. Additional guidance for INTERN supplements can be found in NSF 21-013.

2. EAGER proposals that seek to develop potentially transformational applications of AI that advance one or more MPS domains; EAGER (Early-concept Grants for Exploratory Research) proposals are appropriate in cases where "exploratory work in its early stages on untested, but potentially transformative, research ideas or approaches" will take place. EAGERs provide up to $300,000 in support for up to two years.

3. RAISE proposals that seek to support bold, interdisciplinary approaches that foster MPS discovery using artificial intelligence. RAISE (Research Advanced by Interdisciplinary Science and Engineering) proposals aim for transformational research advances by combining an inherently multidisciplinary approach, and prospective discoveries that "reside at the interfaces of disciplinary boundaries." RAISE projects can request up to $1,000,000 for up to five years.

PROPOSAL PREPARATION AND SUBMISSION

In addition to the standard NSF Proposal & Award Policies & Procedures Guide (PAPPG) guidelines, proposals under this DCL are subject to the following requirements:

- Proposal Title should begin with the type of proposal and "ADAPT:": e.g. "EAGER: ADAPT:" or "RAISE: ADAPT:", as appropriate.
- Supplemental funding requests should mention "ADAPT" and reference this DCL in the summary of proposed work section.
- Before submission of EAGER and RAISE proposals, an up to two-page Research Concept Outline must be submitted to and approved by a DCL cognizant Program Officer.
- Email documentation from at least one DCL cognizant Program Director confirming approval to submit an EAGER (RAISE) proposal must be uploaded as a Supplementary Document entitled "EAGER (RAISE) - Program Director Concurrence Email." A RAISE proposal requires at least two such emails from at least two NSF Program Officers from intellectually distinct programs.

GOALI supplemental funding requests must include a GOALI-Industrial PI Confirmation Letter from the industrial partner that confirms the participation of a co-PI from industry.

Principal Investigators interested in submitting a proposal in response to this DCL are strongly encouraged to contact one of the cognizant Program Directors prior to submission. As noted above, Principal Investigators must contact a cognizant Program Officer prior to submission of an EAGER or a RAISE proposal. A list of cognizant Program Directors can be found below. Full guidance on submitting EAGER, RAISE, or GOALI proposals may be found in Chapters II.E.2-II.E.4 of the PAPPG. Guidance on submitting supplemental funding requests is contained in PAPPG Chapter VI.E.4.

For EAGER and RAISE proposals, a successful research concept outline will describe the following:

- A description of the key concepts of the research to be proposed, including the extent to which they have the potential to transform and impact MPS disciplines, artificial intelligence, or other domains with broader societal impacts.
- The extent to which the proposed work is unique or builds on existing work to make new connections that advance MPS science and/or artificial intelligence.
- For EAGER proposals, the potential to identify new concepts or develop knowledge that can scale up to future larger research activities.
- For RAISE proposals, the extent to which scientific advances lie outside a single MPS program or discipline, and the extent to which prospective discoveries reside at the interfaces of disciplinary boundaries.

For further information on this DCL, please contact one of the following cognizant Program Directors:

- MPS/AST: Dr. Nigel A. Sharp (nsharp@nsf.gov)
- MPS/CHE: Dr. Michel Dupuis (mdupuis@nsf.gov)
- MPS/DMR: Dr. John A. Schlueter (jschluet@nsf.gov)
- MPS/DMS: Dr. Huixia Wang (huiwang@nsf.gov)
- MPS/PHY: Dr. James Shank (jshank@nsf.gov)

Sincerely,

Sean L. Jones,
Assistant Director
Directorate for Mathematical and Physical Sciences