I. Opportunity Description

The Defense Advanced Research Projects Agency (DARPA) is issuing an Artificial Intelligence Exploration (AIE) Opportunity, inviting submissions of innovative basic or applied research concepts in the technical domain of automated knowledge discovery, curation, and application. This AIE Opportunity is being issued under the Program Announcement for AIE, DARPA-PA-18-02. All proposals in response to the Automating Scientific Knowledge Extraction (ASKE) opportunity, as described herein, will be submitted to DARPA-PA-18-02-01. If selected, it will result in an award of an Other Transaction (OT) for Prototype agreement that will not exceed $1,000,000.

A. Introduction

Computational models can elucidate complex systems in a predictive and explainable way, but building them is a laborious process that requires significant manual effort to gather information from experts and implement the model. The resulting models often embody the limitations of the model creator's knowledge and biases. Further, it is rare that scientists and subject matter experts are also expert software engineers so model implementations usually do not follow software development best practices, making them prone to errors and difficult to verify or improve as new information emerges.

B. Objective/Scope

This AIE Opportunity is soliciting proposals to develop approaches to build, maintain, and reason over rich models of complex systems (physical, biological, social, engineered, or hybrid systems) by interpreting and exposing scientific knowledge and assumptions in existing model code and documentation, identifying new data and information resources automatically, extracting useful information (causal relations, correlations, context, parameters, etc.) from these sources, integrating this useful information into machine-curated expert models, and executing these models in robust ways. The resulting models should return rich explanations under a variety of different expert queries, and eventually be capable of generating (and testing by linking to structured data sources) machine-generated hypotheses. Applications of interest include automatic verification of published scientific results and real-time monitoring of fragile economic, political, social, and environmental systems undergoing complex events. Efforts may apply and/or advance AI techniques such as natural language processing, knowledge-based reasoning, machine learning, and/or human-machine collaboration. DARPA's overriding interest is in innovative approaches to extracting knowledge from scientific models.

1. Machine Assisted Curation

Much of the scientific knowledge in the world is encoded most explicitly in scientific model codes. In the physical and biological sciences, this often takes the form of sets of coupled differential equations that are derived from some first principles (e.g. fluid dynamics) or from

empirical observation of aggregate phenomena (e.g., radiation use efficiency in plants). These equations include parameters calibrated to observational or experimental data, which are often updated over the model's lifetime as research produces more data. The structure of the equations must sometimes be updated as well, to correct errors or to include new phenomena that has recently been discovered to be significant (e.g., adding the complex biophysical effects of surface ozone damage to models of plants). Partial automation of this process could dramatically speed up the pace and consistency of scientific discoveries and their application to urgent problems.

2. Machine Assisted Inference

Scientists derive insights from models of complex systems by applying the models to address various types of prognostic queries. This can include, for example:

- *Prediction:* How will the system evolve in the near future?
- *Conditional forecasting:* How will the system respond if X changes?
- *Counterfactual analysis:* What would have happened if X had been Y?
- *Comparative impact:* What is the difference in utility between strategy X and strategy Y?
- *Optimal planning:* What is the optimal amount of X to introduce to maximize utility Y?
- *Risk assessment:* What is the risk of X?
- *Outcome avoidance:* What is the optimal action or intervention to reduce the risk of X decreasing more than Y?

Model-based inference can also be used diagnostically to test models against available data or knowledge through model checking, validation, and calibration. Automation of model-based inference procedures could increase the speed and accuracy with which these models can be used to address key questions of national security by orders of magnitude. Applications will include frequent update of user-specified queries as new data becomes available, rapid response to emerging natural disasters or other real-time threats, and even fully automated inference with machine-generated queries.

C. Structure

Proposals submitted to DARPA-PA-18-02 in response to either of the technical areas (TAs) of this AIE Opportunity must be UNCLASSIFIED, and must address two independent and sequential project phases [a Phase 1 Feasibility Study (base) and a Phase 2 Proof of Concept (option)]. The periods of performance for these phases are 6 months for the Phase 1 (base) effort and 12 months for the Phase 2 (option) effort. Combined Phase 1 base and Phase 2 option efforts for this AIE opportunity should not exceed 18 months. The Phase 1 (base) award value shall not exceed $300,000. The Phase 2 (option) award value shall not exceed $700,000. The total award value for the combined Phase 1 and Phase 2 is limited to $1,000,000. Proposers may address one or both technical areas. Please note that proposers shall address only one TA per proposal.

Phase 1 studies will be evaluated to determine the feasibility of the approach and whether to select the option for Phase 2.

D. Technical Area Descriptions

This AIE Opportunity is interested in efforts that develop and demonstrate an approach to parse and curate models or automate procedures required to perform inference over existing models in scientific domains. Proposals should address one of the following technical areas and its research project objectives.

TA1: Machine-Assisted Curation

TA1 proposals should describe approaches that extract information from scientific model code, documentation, and publications to create, maintain, and update rich semantic representations of scientific models. Proposed approaches should address the following challenges:

1) Automatically identify new relevant processes from the scientific literature (or other sources) and extract causal relations and other information to augment the curated model;
2) Compare representations generated from independent models in the same domain to identify similarities and differences, and demonstrate the capacity to generate meta-models for the domain;
3) Demonstrate the capacity to automatically generate executable code from models modified at the semantic level; and
4) Demonstrate the capacity to extract human-readable explanations of model details, functions, and results.

In addition to the technical details of the approach, proposals to TA1 must specify the scientific domain, and explicitly state the reference scientific models (or journal articles) that will be used to generate semantic representations. The reference scientific model should be open-source, widely used in the specified scientific domain, and sufficiently complex (i.e., have variable declarations, type definitions, loops, sections of well documented code as well as undocumented code, etc.). Approaches should directly address model sensitivity and uncertainty quantification. Approaches that are agnostic to the programming language and enable multi-modal model execution are preferred.

TA2: Machine-Assisted Inference

TA2 proposals should describe approaches that create and apply meta-process-models and ontologies for common model-based inference procedures (e.g., prediction) used in complex systems analysis. Proposed approaches should address the following challenges:

1) Translate expert queries into parameterizations and executions of models;
2) Demonstrate an approach for machine-generation and evaluation of expert hypotheses and diagnostic and prognostic queries;
3) Interpret model outputs to identify novel characteristics or flaws; and
4) Demonstrate the capacity to elaborate human-readable explanations of results from the query and inference procedures.

In addition to the technical details of the approach, proposals to TA2 must specify the scientific domain, and provide examples of how expert queries, diagnostics, and hypotheses will be included in the procedural ontology/meta-model, tested/informed by model executions, and validated. Approaches should directly address model sensitivity and uncertainty quantification.

E. Schedule/Milestones

Proposers must address the following research project objectives, deliverables, and fixed payable milestones in their proposals. The task structure must be consistent across the proposed schedule, Task Description Document (TDD), and the Volume 2 - Price Volume. If selected for award negotiation, the fixed payable milestones provided in Section 9.c of the Volume 2 - Price Volume will be directly incorporated into Attachment 3 of the OT for Prototype agreement ("Schedule of Milestones and Payments"). Please see the sample OT for Prototype agreement provided as an attachment to the AIE Program Announcement (DARPA-PA-18-02).

For planning and budgetary purposes, proposers should assume a program start date of November 1, 2018. Schedules will be synchronized across performers, as required, and monitored/revised as necessary throughout the effort. Proposals must include delivery schedules for Phase 1 and Phase 2 that include timelines for preliminary (to facilitate inspection by the Program Manager) and final (to facilitate evaluation) release of deliverables. Proposals for the ASKE program shall include, at a minimum, the following fixed milestones:

Phase 1 Milestones and Meetings:

Month 1: Report on initial architectures, algorithms, and approaches
Month 3: Interim report describing prototype system
Month 5: Initial code release and final Phase I Report summarizing approach; prototype architectures and algorithms; data sets; results; comparison with alternative state-of-the-art methodology; quantification of accuracy; quantification of robustness

Phase 2 Milestones and Meetings:

Month 6: PI meeting and Milestone Report
Month 7: Report on lessons learned, updated architectures, algorithms and approaches
Month 9: Report describing initial results and proposing evaluation metrics
Month 11: Interim code release and scripted demonstration of system showing performance for real-world system/process and Milestone Report
Month 12: PI meeting and Milestone Report
Month 13: Interim report quantifying system performance, comparing with alternative state-of-the art approaches
Month 15: Live demonstration of system showing performance for real-world system/process and Milestone Report
Month 18: Final code release and Phase II report documenting final prototype architectures and algorithms; methods; results; comparisons with alternative methods; and quantification of accuracy, robustness and generalizability

All proposals must include the following meetings and travel in the proposed schedule and price:

- A two-day kick-off meeting will be held during the Phase 1 base effort, and, to foster collaboration between teams and disseminate ASKE AIE topic developments, two two-day Principal Investigator (PI) meetings will be held during the Phase 2 option effort. For budgeting purposes, plan for three two-day meetings over the course of 18 months: two meetings in the Washington, D.C. area and one meeting in the San Francisco, CA area.

- Regular teleconference meetings will be scheduled with the Government team for progress reporting, as well as for problem identification and mitigation.
- Proposers should also anticipate at least one site visit per phase by the DARPA Program Manager. At that time, performers will have the opportunity to demonstrate progress towards agreed-upon milestones.

F. Deliverables

In addition to the deliverables required for the Phase 1 and 2 milestones, Performers will be expected to provide at a minimum the following deliverables:

- Negotiated deliverables specific to the objectives of the individual efforts. These may include registered reports, experimental protocols, publications, intermediate and final versions of software libraries, code, and APIs, including documentation and user manuals, and/or a comprehensive assemblage of design documents, models, modeling data and results, and model validation data.
- Unless otherwise specified, all deliverables are expected to be released under open-source licenses using standard best practices for versioning and usability.

II. Award Information

Selected proposals that are successfully negotiated will result in award of an OT for Prototype project. See Section 3 of the AIE Program Announcement (DARPA-PA-18-02) for information on awards that may result from proposals submitted in response to this notice.

Proposers must review the model OT for Prototype agreement provided as an attachment to the AIE Program Announcement (DARPA-PA-18-02) prior to submitting a proposal. DARPA has provided the model OT in order to expedite the negotiation and award process, and ensure DARPA achieves the goal of AIE, which is to enable DARPA to initiate a new investment in less than 90 days from idea inception. The model OT is representative of the terms and conditions that DARPA intends to award for all AIE awards. The task description document, schedule of milestones and payments, and data rights assertions requested under Volume 1, Volume 2, and Volume 3 of the AIE Opportunity will be included as attachments to the OT agreement upon negotiation and award.

Proposers may suggest edits to the model OT for consideration by DARPA and provide a copy of the model OT with track changes as part of their proposal package. Suggested edits may not be accepted by DARPA. The Government reserves the right to remove a proposal from award consideration should the parties fail to reach agreement on OT award terms and conditions. If edits to the model OT are not provided as part of the proposal package, DARPA assumes that the proposer has reviewed and accepted the award terms and conditions to which they may have to adhere and the sample OT agreement provided as an attachment, indicating agreement (in principle) with the listed terms and conditions applicable to the specific award instrument.

III. Eligibility

See Section 4 of the AIE Program Announcement (DARPA-PA-18-02) for information on who may be eligible to respond to this notice.

IV. AIE Opportunity Responses

Responses to this AIE Opportunity must be submitted as full proposals to DARPA-PA-18-02as described therein. All proposals must be UNCLASSIFIED.

A. Proposal Content and Format

All proposals submitted in response to this notice must comply with the content and format instructions in Section 5 of the AIE Program Announcement (DARPA-PA-18-02). All proposals must use the templates provided as attachments to the PA and follow the instructions therein.

Information not explicitly requested in the AIE Program Announcement (DARPA-PA-18-02), its attachments, or this notice) may not be evaluated.

B. Proposal Submission Instructions

See Section 5 of the AIE Program Announcement (DARPA-PA-18-02) for proposal submission instructions.

C. Proposal Due Date and Time

Proposals in response to this notice are due no later than **September 17, 2018 at 4:00 p.m. (ET)**. Full proposal packages as described in Section 5 of the AIE Program Announcement (DARPA-PA-18-02) must be submitted per the instructions outlined therein *and received by DARPA* no later than the above date and time. ASKE AIE Opportunity proposals received after this date and time may not be reviewed.

Proposers are warned that submission deadlines as outlined herein are in Eastern Time and will be strictly enforced. When planning a response to this notice, proposers should take into account that some parts of the submission process may take from 1 business day to 1 month to complete.

V. Proposal Evaluation and Selection

Proposals will be evaluated and selected in accordance with Section 6 of the AIE Program Announcement (DARPA-PA-18-02). Proposers will be notified of the results of this process as described in Section 7.1 of that same announcement.

VI. Administrative and National Policy Requirements

Section 7.2 of the AIE Program Announcement (DARPA-PA-18-02) provides information on Administrative and National Policy Requirements that may be applicable for proposal submission as well as performance under an award.

VII. Point of Contact Information

Joshua Elliott, Program Manager, DARPA/I2O, ASKE@darpa.mil

VIII. Frequently Asked Questions (FAQs)

All technical, contractual, and administrative questions regarding this notice must be emailed to ASKE@darpa.mil. Emails sent directly to the Program Manager or any other address may result in delayed or no response.

All questions must be in English and must include name, email address, and the telephone number of a point of contact. DARPA will attempt to answer questions publically in a timely manner; however, questions submitted within 7 days of the proposal due date and time listed herein may not be answered.

DARPA will post an FAQ list under the AIE Opportunity on the DARPA Opportunities page at https://www.darpa.mil/work-with-us/opportunities?tFilter=&oFilter=3&sort=name. The list will be updated on an ongoing basis until one week prior to the proposal due date and time. In addition to the ASKE AIE Opportunity FAQ, which is specific to this notice, proposers should also review the general AIE FAQ list at https://www.darpa.mil/work-with-us/opportunities?PP=2.