# Multi-AI Capable Cyberinfrastructure

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### White Paper for Workshop on Next Generation of Smart Cyberinfrastructure

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This White Paper will provide a viewpoint on (1) how scientific cyberinfrastructure will need to evolve to better support a wider range of Artificial Intelligence (AI) techniques and methodologies (which I call Multi-AI-Capable), and (2) example uses for Multi-AI-Capable Cyberinfrastructure in scientific discovery.

### Scientific Cyberinfrastructure to Better Support a Wider range of AI Techniques & Methodologies

Existing NSFCloud infrastructures such as CloudLab and Chameleon as well as commercial cloud providers such as Azure and Amazon Web Services (AWS) are rapidly adding hardware optimized for machine learning and classification of patterns. These include fast, parallel, and narrow graphics processing units (GPUs), tensor processing units (TPUs), and smart network interface controllers (smart NICs) among others. There continues to be rapid evolution of hardware optimized for specific uses and keeping up with application-based requirements is a key challenge for both NSF Cloud and commercial providers.

Most the newest and fastest supercomputers are also incorporating architectures designed to facilitate AI workloads. The Japanese AI Bridging Cloud Infrastructure (ABCI) is #8 on the current TOP500 list, but this list ranks by the traditional High Performance Linpack (HPL) benchmark and doesn’t measure true AI capabilities. Both next-generation Chinese and European supercomputers will have internal connectivity and augmented and adjunct processors friendly to multi-dimensional AI problems. Two examples are the Vector Neural Network Instructions (VNNI) in current and future Intel Xeon CPUs, and continuous new takes on tensor co-processors.

To date, most AI algorithms and cyberinfrastructure rely on just two related AI techniques: machine learning of patterns and classification based on those patterns. This white paper argues not that these are unimportant—indeed, they are critically important—but that future AI applications will also rely on additional AI-related cyberinfrastruture capabilities as well. Generically, I call this broader set of capabilities “Multi-AI Capable Cyberinfrastructure.”

Multi-AI Capable Cyberinfrastructure will better support:

* Traditional symbolic AI reasoning and ontological reasoning
* Being able to explain why learning and classification networks are constructed the way they are
* Game-theoretical extrapolations and predictions (leading to better machine and human decision-making)
* AI-driven automatic big data exploration and discovery and testing these results against independent datasets
* Evolutionary and genetically-driven AI capabilities
* Quantum computing support for better probabilistic AI applications (Quantum wave function superpositioning might be used to represent probabilistic certainties (aka “uncertainties”) in AI algorithms)

Each of these bullets deserves a paragraph to explore their importance and possible approaches to cyberinfrastructure to better support them. But let’s leave that to a workshop report that covers those (and others) on which we have a degree of agreement.

### Multi-AI-Capable Cyberinfrastructure in Scientific Discovery

There would appear to be a very long list of possible applications for Multi-AI-Capable Cyberinfrastructure in Scientific Discovery. Before listing some of these, let’s just note that we’re omitting big classes of applications which have already received significant attention such as military applications, autonomous vehicles, digital assistants, traffic management, social media, interpreting medical imaging, financial investing, etc. And we’re not claiming these are already solved; just that we’re likely to make more of an NSF difference by focusing on some important issues in science.

How might Multi-AI Capable Cyberinfrastucture better support science and engineering?

1. Intelligent agents to facilitate use of the Scientific Method. An AI-based digital lab assistant could help support documentation of the environment, hypotheses, helping with experimental design to maintain desired power in the results, accurately recording experiments (including those run on Multi-AI Capable Cyberinfrastructure), and aiding reproducibility and replicability. “Reproducibility and Replicability in Science” was the title of a Congressionally-required, NSF-commissioned report by the National Academies of Science and Engineering released May 7th,. Using Multi-AI Capable Cyberinfrastructure to better design and document scientific hypotheses and experiments could have great value across all NSF directorates.
2. Creation, testing, and tuning of scientific models / simulations / emulations / cyberphysical systems. The Wikipedia article on Artificial Intelligence notes that “Leading AI textbooks define the field as the study of "[intelligent agents](https://en.wikipedia.org/wiki/Intelligent_agent)": any device that perceives its environment and takes actions that maximize its chance of successfully achieving its goals.” (See English Wikipedia for references.) I would suggest that models (and simulations and emulations and self-adjusting cyberphysical systems) are key to many areas of science. A grand challenge might be a National Library of AI-driven Scientific Models. Many AI-driven topic-specific models already exist. But they are few compared to the number of topic-specific models carefully constructed by knowledgeable scientists and engineers. Multi-AI techniques could be the key to greatly expanding the breadth and number of useful models and helping them evolve to match new data. Which brings us to…
3. Discovery in data that goes beyond simple patterns and looks for multi-step explanations and interactions. How are time-varying complex patterns related to each other? Can Multi-AI-Capable Cyberinfrastructure help with model verification? Model-driven prediction? Model tuning? Model explanation?
4. Cybersecurity research is a constantly evolving subject that might be viewed as based on game theory. Multi-AI-Capable Cyberinfrastructure designed for game theory applications could help produce significant new results in cybersecurity.
5. Both student-directed and Socratic learning digital assistants. Today’s dominant uses of linear textbooks, syllabus-based lectures, and educational projects work for some but not all learners. The National Science Foundation has an important interest in science and technology education that might better be achieved for some students with experience-inspired student-directed learning. Can Multi-AI-Capable Cyberinfrastructure re-structure learning materials on the fly to meet the needs of a learner’s question? Similarly, the Socratic Method is often very effective for some students but not widely used for teaching science and engineering. How could a Multi-AI-Capable Cyberinfrastructure ask probing questions, understand the student’s thinking based on their response, and then ask additional questions that lead the student to the answers they seek? (Another grand challenge.)
6. Smart and Connected Communities research could widely benefit from Multi-AI-Capable Cyberinfrastructure. A quick listing of example applications that would benefit from Multi-AI Capable techniques includes:
	1. Anticipating human needs (e.g. public safety, transportation, health)
	2. Consumer-driven AI to make it an even fight with marketing-driven AI (information asymmetry)
	3. Continuous health monitoring
	4. Robotic companions for seniors
	5. Advising citizens on changing existential habits (uses of energy, water, etc.)
	6. Micro transit coordination
	7. Micro grid coordination
	8. Countering social media addiction
	9. Ethical AI; where AI intersects with people, we can’t ignore the ethics