NSF Smart Cyberinfrastructure Workshop White Paper:

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Title: "Features of a Possible NSF Smart Cyberinfrastructure Roadmap Supporting Science Applications"

Focus: Associated needs & requirements with illustrative exemplar application from Fusion Energy

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The basic motivation behind NSF's strong current interest in developing a "Smart Cyberinfrastructure (CI) Roadmap" is to appropriately address the challenge of integrating emerging new smart technologies in Artificial Intelligence/Deep Learning/Machine Learning into existing and future scientific investigations involving the synergistic engagement of the Agency's CI and applications communities. This process can begin by moving toward a common understanding of the current and evolving requirements of "Smart CI" in terms of architectures, algorithms, best practices, enabling technologies, and current gaps in CI for the present and near future,

While there is abundant evidence of great national and international enthusiasm for launching major AI-centric new R&D programs, a logical starting point is to address the following basic set of 6 associated questions: (1) What exciting grand challenge problems can best be addressed with AI-enabled cross-disciplinary cyberinfrastructure" ?; (2) What transformational ideas for associated efficient coupling of simulations, experiments, & computing facilities are needed to accelerate progress in scientific discovery?; (3) What kinds of modern computer architectures and associated infrastructure can best serve the needs of AI-enabled discovery science ?; (4) Since the coupling of AI and HPC is a well-recognized to be a huge opportunity for AI-enabled cyberinfrastructure, what approaches should be adopted ? (6) How can we best enhance exciting opportunities for international and industrial collaborations in an AI-enabled ecosystem?

We can begin by considering some guiding principles for possible NSF Cross-Disciplinary AI Institutes with key themes that include, for example: (1) Trustworthy AI; (2) Foundations of Machine Learning; and (3) AI for Discovery in Physics. The overall, targeted work-scope should cover both foundational as well as "use-inspired" AI research to be explored. Another key element of such interdisciplinary computational institutes would be to further strengthen NSF's mission for education & training of current and future generations of the US workforce -- with the skills to develop and apply AI tools and technologies with innovative impact on today's economy and jobs of the future. This would of cource focus on AI-enabled approaches for education and development of the Nation's graduate and undergraduate students, post-doctoral researchers, and skilled technical workforce. Associated NSF Cross Disciplinary AI institutes could involve universities as well as NSF supercomputing centers (e.g., SDSC, TACC, NCSA, …) who would be well positioned to conduct courses in Deep Learning/Machine Learning with associated connections to workshops and "hackathons" for enabling timely assimilation of new concepts and methodologies in AI-enabled discovery science. The institutes should also be encouraged to engage and establish attractive connections to leading industries – such as Microsoft, Nvidia, Intel, Google-Brain, & Facebook -- to help inject an exciting level of practical connections to accelerated deployment of modern technology.

It is important to create a sense of excitement that requires identifying scientific applications that motivate/energize creation of such a new NSF Smart Cyberinfrastructure. For example -- CNN's "MOONSHOTS for 21st CENTURY" (Hosted by Fareed Zakaria) – has identified 6 grand challenge areas that are easily understandable to the general public to be hisworthy enterprises to be targeted. Fusion Energy is a compelling exemplar in this set, and an associated inspirational endorsement from Stephen Hawking came from his BBC Interview, 18 Nov. 2016, where he commented: "I would like nuclear fusion to become a practical power source. It would provide an inexhaustible supply of energy, without pollution or global warming."

At this point, we will now focus for the rest of this White Paper on using Fusion Energy as an exemplar for illustrating associated needs and requirements associated with “Smart Cyberinfrastructure.” Here the major grand challenge involves the demonstration of the scientific and technological feasibility of delivering fusion power in the multinational ITER project – with the highest priority being to accurately predict & control disruptions for the $25B burning plasma ITER experiment that has the goal of exceeding “break-even” (or “power in = power out”) by a factor of 10 to 20.

<u>What can AI-enabled advanced cyberinfrastructure deliver today in this Exemplar area?</u>

Artificial Intelligence/Deep Learning brings new technology to accelerate progress
"Predicting Disruptive Instabilities in Controlled Fusion Plasmas through Deep Learning”
NATURE: April, 2019 : Princeton’s Fusion Recurrent Neural Network code (FRNN) uses convolutional & recurrent neural network components to integrate both spatial and temporal information for predicting disruptions in tokamak plasmas with unprecedented accuracy and speed on top supercomputers worldwide.

Things we can do in FES with AI now & on near term horizon in this Exemplar area include:
i) Learn predictive models from data without relying upon analytic theory or deep mechanistic understanding: Example: predicting dangerous disruptive events in tokamaks using AI/Deep Learning on huge measured data base enabled by training on leadership class supercomputers achieving unprecedented accuracy and speed.
ii) Initiate moving from prediction to active real-time plasma control:
Example: Introduce a “software integration wrapper” enabling conversion of deep learning predictors written in modern Python/Keras language into conventional plasma control systems written in the older C language.
iii) Develop new software to help explain reasons for deep learning predictive accuracy:
Example: Introduce capability to output not only the “disruption score” for the probability of a disruption event but also a “sensitivity score” in real-time to indicate the underlying physics reasons for the Imminent disruption. ➔ physics-based interpretability + targeted guidance for control actuators upon Implementation into a modern plasma control system (PCS).
Iv) Carry out convergence studies of HPC advances with DL/AI predictive workflow:
Example: First obtain realistic pre-disruption classifiers (e.g. for experimentally-observed “neoclassical tearing modes) from “reduced models” derived from 1st-principles-based electromagnetic PIC simulation results carried out on the SUMMIT supercomputer using exascale class GTC code – and then insert into the AI/DL workflow.

<u>What can AI-enabled advanced cyberinfrastructure deliver within 5 years in this Exemplar area?.</u>

• Successful Development of:
i) Efficient & realistic control strategies based on advanced AI/DL predictors emerge for optimization of performance and avoidance of disruptions in initial operations of ITER;
ii) Continuous vetting of stable, scalable, portable control systems and associated methodology on existing tokamaks (e.g., DIII-D, JET, KSTAR, … leading to the large superconducting JT60-SA tokamak in Japan and finally to ITER)
Cross-disciplinary Exploration:
iii) Novel real-time control methods learned from expertise residing in application areas such as robotics and self-driving cars;
→ Enables leveraging vast experience from well established institutions, including (e.g., Alan Turing Institute in UK); active industrial engagement, such as Microsoft, NVIDIA, INTEL, GOOGLE, FACEBOOK, …..)
• Automation & Acceleration of Discovery Science:
• Systematically moving from (i) New Planning, to Creative Conjecture, to (ii) Further

Experimentation, to (iii) Confirmation/Validation and Integration of New Analysis
➔ Vision of "End-to-End" automated harvesting of real-time scientific insights from operating modern experimental facilities

What can AI-enabled advanced cyberinfrastructure deliver after 10 years in this Exemplar area?

• Realistic real-time models to reduce actual numbers of necessary experiments as the experiments incorporate "lessons learned" from such AI-enabled higher physics fidelity models
• AI becomes common part of scientific laboratory activities.
• AI infuses new scientific, engineering, and operations methodologies into FES
➔ Development of "Virtual Experiments" emerging from validation vs. large trustworthy data bases with associated sensitivity testing to provide an essential filter against "over-hyped" claims
• Improved theoretical formulations from integration of new AI/DL-enabled statistically-validated insights to long-standing plasma physics/FES theories remove/reduce problematic/uncertainty areas
• Validated theory becomes data source for next-generation AI in FES, so that AI begins to contribute to advancing fundamental Plasma Physics/FES theory
• AI-enabled in-depth pursuit of creative FES physics scenarios – e.g., advanced materials, such as, high-temperature superconducting large magnetic field to enable modularity and compactness.

Concluding Comments/Observations on Impact of AI-enabled Advanced Cyberinfrastructure:

• The rapid growth of AI/DL/AI in prominent application domains are likely to mirror the revolutionary trends seen in the business world today – e.g., the re-formation of Amazon and other top businesses that have incorporated AI/DL/ML
https://www.wired.com/story/amazon-artificial-intelligence-flywheel/

• Cross-disciplinary engagement can yield accelerated mutually beneficial results (e.g., Cancer & Clean Energy Fusion R&D)

- Cancer Research → Reference: "Candle Project" with ECP Exascale Computing Project (DOE & NIH) to identify optimal cancer treatment strategies, by building a scalable deep neural network code called the CANcer Distributed Learning Environment (CANDLE).
- → development of predictive models for drug response, and automation of the analysis of information from millions of cancer patient records -- via developing, implementing, & testing DL/AI Algorithms and their benchmarks – such as hyperparameter tuning and associated complex workflows

- → development of predictive models (as just illustrated) in Clean Fusion Energy R&D have followed similar AI/DL approaches

➔DL/AI advances in very different key application Grand Challenge areas like Clean Energy Fusion and Cancer Research can stimulate enhanced cross-disciplinary efforts to leverage connections to enormous worldwide investments in AI/DL/ML R&D !