Research in artificial intelligence (AI) is of significant interest because of the vast potential of AI technology to impact or completely transform many sectors within society. Recent advances in AI such as speech, image, and facial recognition, as well as language translation, are already showing up in smart technology and will continue to be utilized as AI continues to advance. Industry is already using AI to optimize processes, design better components, and increase efficiencies, all the while looking for more ways to streamline operations using AI. And on the materials front, the use of AI and machine learning (ML) are already being employed to accelerate materials discovery and design.*

While the US federal government has long supported fundamental research in AI, the 2019 update to the 2016 National Artificial Intelligence Research and Development Strategic Plan identified a need to make longer-term investments in AI research. According to the updated AI Strategic Plan, much of the AI research to date has been specialized around specific tasks, and longer-term investments are needed to expand and broaden AI into “systems that exhibit the flexibility and versatility of human intelligence in a broad range of cognitive domains.”

In October 2019, the US National Science Foundation (NSF) cited the updated AI Strategic Plan’s call for longer-term investments in AI research when announcing the creation of a new interagency program to establish AI research institutes. The National Artificial Intelligence Research Institutes program will spend up to USD$124 million and provide funding for up to eight planning grants (up to two years and USD$500,000) and between one and six AI Research Institutes (4–5 years at up to USD$4 million/year). Initial areas of focus include trustworthy AI, foundations of ML, AI-driven innovation in agriculture and the food system, AI-augmented learning—and most relevant for materials research—AI for accelerating molecular synthesis and manufacturing, and AI for discovery in physics.

The creation of this program ensures a shift from traditional short-term funding of two years to long-term investment in AI research. The NSF’s grant solicitation acknowledges this fact stating, “Among Federal research investments, institute-scale activities enable multidisciplinary, multi-stakeholder teams to focus on larger-scale, longer-time horizon challenges…”

“Sustained, longer-term funding [in AI] is most welcome,” says Kristofer Reyes, assistant professor of materials design and innovation at the University at Buffalo, The State University of New York. Reyes adds, “I think this would allow our community to take a more strategic perspective when it comes to the application of AI/ML to materials, rather than one-off demonstrations of off-the-shelf techniques.”

Benji Maruyama, Flexible Materials and Processes Research Team Lead in the Materials and Manufacturing Directorate at the Air Force Research Laboratory, agrees and points out, “materials research can complement AI research by providing valuable challenge problems to test ideas on AI/ML approaches.” According to Maruyama, materials researchers can readily provide “data streams of experimental and simulated data,” which Reyes says could be used to determine how well “problem-agnostic ML/AI methods” can adapt to a variety of data types and sources.

Credit: Photo by Andrew Kelly/New York Hall of Science.

*For an in-depth discussion of recent advances, industry uses, and materials-specific uses of AI and ML, see the July 2019 issue of MRS Bulletin.

---

**AI** artificial intelligence: the ability of computers to mimic the cognitive function of humans

**ML** machine learning: a subset of AI where computers apply data/information to independently update algorithms during processing; essentially the ability of the computer to learn from the data/input and adjust accordingly.
Both Reyes and Maruyama also agree that AI, and more specifically ML, are poised to have a significant impact on materials research. “I think the most immediate impact of the use of ML in materials is the ability to train models that can predict materials properties and performance from an appropriate set of features,” Reyes says, which will enable researchers to discover new and better materials options, and could be used to guide experiments and increase research efficiency. Maruyama adds, “using AI/ML approaches enables us to analyze and hopefully extract meaning from complex, interdependent, high-dimensional problems that are increasingly relevant as our experimental tools generate more and more complex data streams.”

AI-enabled materials research holds substantial promise beyond modeling and predicting, though. “One of the aspects of AI and ML that I am most looking forward to is the increasing use of natural language processing to sift through materials research and extract information and knowledge,” Reyes says.

And Maruyama highlights current work in Autonomous Research, which he says, “exploits AI algorithms via autonomous research robots that do rapid, closed-loop experimentation.” This means that the research robots can execute experiments, vary parameters, and characterize the results without human intervention. According to Maruyama, “Autonomous Research systems will lead to an exponential explosion in research progress, akin to Moore’s Law for the speed of research.”

While dedicated, long-term AI research is clearly important, Reyes expresses concern that past calls to fund interdisciplinary AI/ML research have “required novelty in both the AI/ML aspect as well as the materials aspect,” which he says is too ambitious. “I believe the application of AI/ML to materials is research in and of itself,” he says.

Maruyama concurs: “We should think about how AI/ML improve the speed, depth, and productivity of research.” Maruyama characterizes this type of research as a movement to advance how research is conducted, which is often overlooked as it does not comply with the usual nature of basic research.

Maruyama points out that “AI will help us make better and faster decisions about how to interpret and act on data,” and he expresses hope it will be funded by the AI research institutes because of the “fundamental changes it will bring to our research processes.”

One other critical area the AI research institutes will need to address, according to Reyes and Maruyama, is how they will prepare researchers to work in this field. The AI Research Institutes grant solicitation makes it clear that this is also one of the program goals, saying that the AI Research Institutes will “actively build the next generation of talent for a diverse, well-trained workforce.”

Jennifer A. Nekuda Malik

---

**European Commission funds startups and SMEs to shape the future**

Seventy-five startups and SMEs have been selected in the largest funding round so far under the pilot phase of the European Innovation Council (EIC) Accelerator. Among the companies selected is Chrysalix Technologies in Estonia, a university spin-off producing sustainable fuel using organic material; Solenco Power NV in Belgium, to provide solar power nonstop on or off the grid; and Recresco Limited in the UK for the development of x-ray fluorescence, shape recognition, and machine learning for efficient and economic recycling of mixed metals from co-mingled waste.

As a major novelty, 39 of these companies are set to receive both a grant and a direct equity investment. This is the first time that this “blended finance” has been offered, and it allows a much higher level of funding (up to €17.5 million per company) to accelerate the growth of European companies with groundbreaking innovations.

Mariya Gabriel, Commissioner for Innovation, Research, Culture, Education and Youth, said, “I am glad that this first offer of combined grant and equity financing saw such a high demand from Europe’s startups and SMEs. This confirms that the European Innovation Council is filling a gap in funding, and that it is right to set it up as a fully fledged initiative under the next EU budget.”

As well as the financial support, the startups and SMEs will have access to coaching, networking, and business acceleration services to help them build their businesses.