Argonne
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WATER
STRATEGIC PLAN
October 2020

ARGONNE NATIONAL LABORATORY
DECADAL WATER STRATEGY 2020 – 2030
Water science and engineering empowered by artificial intelligence (Water + AI)

Water + AI at Argonne

Argonne leverages multi-disciplinary teams, world-class facilities, powerful scientific tools, and strategic partnerships to confront some of the most profound scientific and technological challenges for water-related science.

Water is our most valuable resource, impacting people, infrastructure, and industries around the globe. As warming temperatures, changes in precipitation and runoff, extreme weather, pandemics, and rise in sea level continue to create new challenges, there is an urgent need for scientific and engineering solutions. Over the next decade, we at Argonne National Laboratory plan to enhance our leadership in this space through pioneering research, discoveries, and innovations in the following areas:

- Water-related materials discovery, synthesis, characterization, and scale-up manufacturing
- New process technologies for systems that sense, treat, and handle water
- Machine learning and artificial intelligence, data science, modeling, and simulation related to new water materials and process technologies

Our strategy is intended to lead to water-based intelligent systems for fit-for-purpose water treatment and distribution, water-enabled energy production, and the sustainable management of all our water resources (see Figure 1). The societal benefit would be to secure America's water resources and deliver economic growth.

Argonne's Vision for the Future

Our vision for the future is that the U.S. Department of Energy (DOE) and the external community will view Argonne as a leading organization for research and innovation in Water Science and Engineering empowered by Artificial Intelligence (Water + AI). In developing our decadal Water + AI strategy for realizing this vision, we gathered data and feedback by conducting town hall meetings (140 attendees), one-on-one and working group meetings (over 200 attendees), and numerous meetings with Argonne division directors and associate laboratory directors, industrial partners, program managers, and other stakeholders. We also based the strategy on the priority research directions laid out in *Basic Research Needs for Water and Energy* (DOE Office of Science) and the goals set forth in the *Water Security Grand Challenge* (DOE Office of Energy Efficiency and Renewable Energy). Argonne staff had leadership roles in producing the *Basic Research Needs* report and participated in framing the *Water Security Grand Challenge*.

With its partners in Chicagoland and beyond, Argonne is ideally suited to take materials and process technologies from discovery to application by tapping into our world-class materials and chemistry expertise, analytical capabilities at the Advanced Photon Source (APS), high-performance computing at the Argonne Leadership Computing Facility (ALCF), nanoscience and nanotechnology capabilities at the Center for Nanoscale Materials (CNM), and scale-up manufacturing capabilities at Argonne's Materials Engineering Research Facility (MERF). The APS, ALCF, and CNM are U.S. Department of Energy Office of Science user facilities at Argonne.
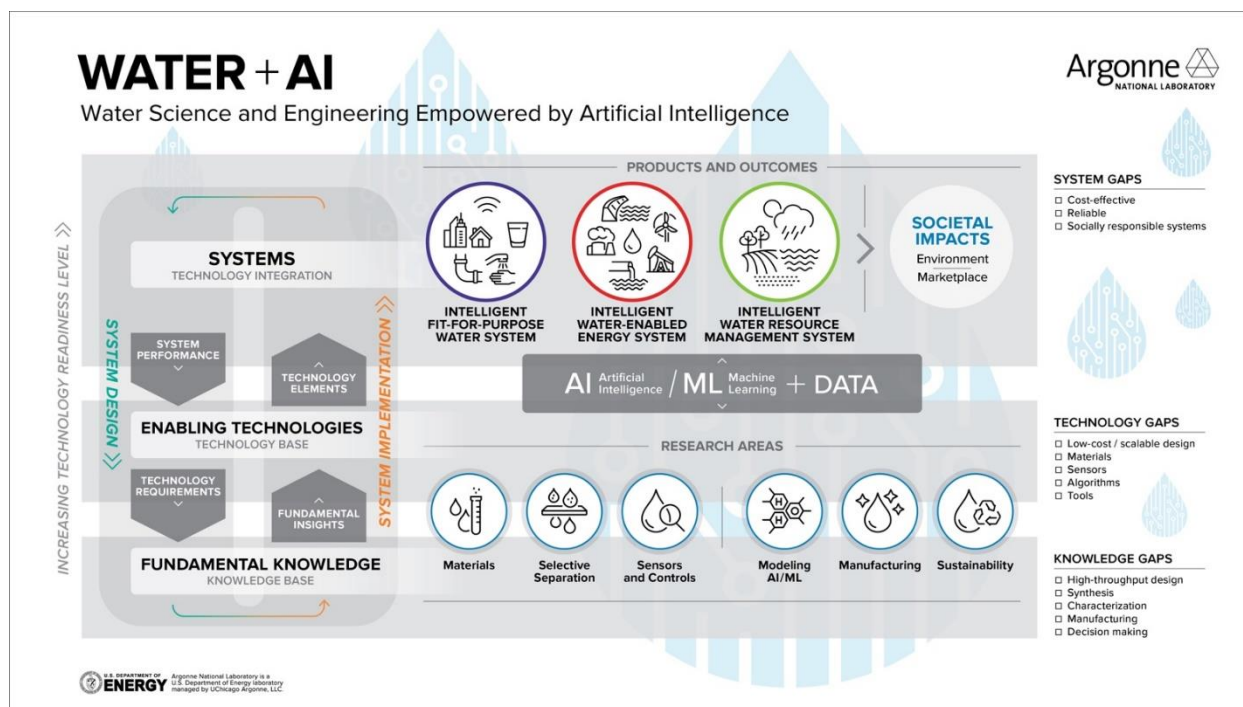
Figure 1: Argonne's ten-year Water + AI strategy.

Global Water Challenges

Without water there is no life. Water is continually cycling through extraction from the environment, then use and return to the environment. Today this cycle is under threat due to many factors, including climate change, increased pollution, skyrocketing demand, and wasteful use. Researchers from around the world are searching for innovative solutions to make this cycle more effective and efficient and help secure a plentiful and clean water supply.

The Argonne Water + AI Strategy

Vital to our nation's future are innovative systems for fit-for-purpose water treatment and distribution, water-enabled energy production, and the sustainable management of all our water resources. The ten-year Water + AI strategy has three elements: developing a fundamental knowledge base in six focus areas, developing enabling technologies in those same areas, and integrating the two in the creation of intelligent water-related systems (see Figure 1). Research programs can start with developing fundamental knowledge and advance to one of the systems, or start with the requirements for a particular system and then develop the needed enabling technologies and fundamental knowledge.

Argonne projects underway or planned in the six focus areas are as follows:

- **Materials.** Argonne's water-related materials projects focus on developing and characterizing various materials such as membranes, sorbents, and catalysts relevant to water monitoring, treatment, conveyance and reuse, and water-enabled energy production. This research area involves high-throughput design of water materials, study of material surfaces and material-water interfaces, and development of selective molecular probes.

- **Sensors and Controls.** In this area, Argonne is developing affordable chemical and biological sensors that monitor water quality in polluted areas and control methods for water-related processes, such as fouling of surfaces. This area includes novel sensing modalities and materials, sensing mechanisms, analyte-probe interactions, and actuation/control methods.

- **Selective Separation**. This focus area involves developing functional groups, sorbents, membranes, and catalysts for selective separation of various contaminants from water. The contaminants span a wide range: heavy metals such as lead, bacteria and viruses, per- and polyfluoroalkyl substances (PFAS), radioactive elements, oil and other petroleum products, and pharmaceuticals. Key here is investigating water science for adsorption and separation, surface reactivity, and transport phenomena in confined spaces.

- **Modeling and Machine Learning (ML)/Artificial Intelligence (AI).** Projects in this area focus on developing accurate and efficient physics-based models and ML/AI algorithms and simulation software to advance the study of water and aqueous solutions. We use these tools to determine the physical and chemical properties of the water-material/contaminant interface at the atomic and molecular scale.

- **Manufacturing.** This focus area concerns the scaleup of materials manufacturing and processing, including data-enabled cyber-manufacturing. It includes development of manufacturing tools and improvement of the manufacturing infrastructure related to water treatment and monitoring, as well as water-enabled energy production.

- **Sustainability.** This focus area's projects employ life-cycle assessment, techno-economic analyses, and risk analyses (socioeconomic and environmental) to ensure our nation's water sustainability. These analyses include resilience and impact evaluation of new water-based technologies during extreme events and pandemics, as well as determination of the social implication of these technologies.

The knowledge base and enabling technologies established in these six focus areas will serve as the springboard for development of three water-related systems essential to securing America's water resources and delivering economic growth:

- **Intelligent fit-for-purpose water systems.** Such systems would provide water of the required quality and quantity to meet demand as it is needed. This would involve selective separation of water contaminants and connection of water treatment plants to sensors along the distribution line, smart water meters and filters, and a user interface tied to wireless data collection and analysis.

- I**ntelligent water-enabled energy systems.** Such systems would make more intelligent use of the cooling and wastewater in power plants, the water involved in hydropower projects and the high-pressure water mixtures in fracking. Water power resource managers, for example, need advanced modeling tools to simulate the potential impacts and value of hydropower projects that would expand the use of renewable energy and its integration into flexible, reliable power grids. In addition, better methods are needed for recovering resources for beneficial uses of the waste water in energy systems.

- **Intelligent management systems for our water resources.** Such systems would more intelligently manage groundwater, surface water, wastewater, and water in polar regions and the atmosphere. By identifying typical sources and distribution of microbial communities in waterways, for example, researchers can develop hydrological models that incorporate the microbial data, laying out how water flows from different sources and how rain events affect bacterial diversity and count.

We will be demonstrating system-level testbeds for the above through control/remediation of various emerging contaminants, such as PFAS, microplastics, and hydrocarbons (e.g., in fracking water) or through resilience in infrastructure or under emergency/extreme situations such as the COVID-19 pandemic.

This strategy covers the entire innovation spectrum from fundamental research to enabling technologies and integrated systems that will impact society in terms of both economic growth and environmental improvements. It draws upon Argonne's strengths in water science and engineering, unique ML/AI capabilities, and world-class scientific facilities such as the APS, ALCF, CNM, and MERF. Finally, it is aligned with (1) the Argonne 2050 strategy; (2) relevant Argonne initiatives (current and past); (3) Argonne's existing strengths in materials, manufacturing and computation, including ML/AI; (4) Argonne's world-class facilities; and (5) Argonne's existing major water efforts in the six areas. Examples of the latter include the research being done in the Advanced Materials for Energy-Water Systems Center—a DOE Energy Frontier Research Center at Argonne—and the Collaborative Water-Energy Research Center—a U.S.-Israel Energy Center.

The Water + AI Strategy: A Case Study

Argonne has initiated a Water + AI program in applying AI to the tracking and remediation of a contaminant in water, PFAS. Remediation of PFAS represents a national grand challenge with high complexity and a large societal impact. At present, there are limited PFAS toxicity data and no effective approaches to track and remove PFAS from water. There are thousands of PFAS compounds; these substances can be found in food, commercial household products, cookware, workplace, living organisms, drinking water, and groundwater. They pose a significant national challenge in terms of detrimental health effects and water reuse, and the estimated cost of national cleanup is in the billions of dollars.

In this new program, Argonne will be exploiting the power of AI and the large databases for PFAS to better understand its complex interactions with water. Without AI, the enormous amounts of data and the large number of PFAS compounds are difficult for humans to fully comprehend or build comprehensive first-principles physics models from them. Argonne will be applying the Water + AI approach to develop models to understand the toxicity of PFAS in water and predict its distribution in water across the nation. Argonne is looking to partner with the U.S. Environmental Protection Agency to fill large gaps with regard to PFAS toxicity and tracking in its databases. The Water + AI approach will also be followed in developing molecular probes that selectively bind PFAS for detection and remediation purposes. Once established, this approach will be applicable to solving similar problems with other emerging contaminants, such as pharmaceuticals in our drinking water, microplastics prevalent in our environment, and hydrocarbons in fracking water.

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ARGONNE NATIONAL LABORATORY

▫ U.S. Department of Energy research facility

▫ Operated by the University of Chicago

▫ Midwest's largest federally funded R&D facility

▫ Located in Lemont, IL, about 25 miles (40 km) southwest of Chicago, IL (USA)

▫ Conducts basic and applied research in dozens of fields

▫ Unique suite of leading-edge and rare scientific user facilities

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