Mitsui and NVIDIA Announce Japan's First Generative AI Supercomputer for Pharmaceutical Industry

Leading pharma companies in Japan will use the Tokyo-1 NVIDIA DGX supercomputer to accelerate drug discovery.

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Mitsui & Co., Ltd., one of Japan's largest business conglomerates, is collaborating with NVIDIA on Tokyo-1 — an initiative to supercharge the nation's pharmaceutical leaders with technology, including high-resolution molecular dynamics simulations and generative AI models for drug discovery.

Announced today at the NVIDIA GTC global AI conference, the Tokyo-1 project features an NVIDIA DGX AI supercomputer that will be accessible to Japan's pharma companies and startups. The effort is poised to accelerate Japan's $100 billion pharma industry, the world's third largest following the U.S. and China.

"Japanese pharma companies are experts in wet lab research, but they have not yet taken advantage of high performance computing and AI on a large scale," said Yuhi Abe, general manager of the digital healthcare business department at Mitsui. "With Tokyo-1, we are creating an innovation hub that will enable the pharma industry to transform the landscape with state-of-the-art tools for AI-accelerated drug discovery."

The project will provide customers with access to NVIDIA DGX H100 nodes supporting molecular dynamics simulations, large language model training, quantum chemistry, generative AI models that create novel molecular structures for potential drugs, and more. Tokyo-1 users can also harness large language models for chemistry, protein, DNA and RNA data formats through the NVIDIA BioNeMo drug discovery software and service.

Xeureka, a Mitsui subsidiary focused on AI-powered drug discovery, will be operating Tokyo-1, which is expected to go online later this year. The initiative will also include workshops and technical training on accelerated computing and AI for drug discovery.

According to Abe, Japan's pharmaceutical environment has long faced drug lag : delays in both drug development and the approval of treatments that are already available elsewhere. The problem received renewed attention during the race to develop vaccines during the COVID-19 pandemic .

The nation's pharmaceutical companies see AI adoption as part of the solution — a key tool to strengthen and accelerate the industry's drug development pipeline. Training and fine-tuning AI models for drug discovery require enormous compute resources, such as the Tokyo-1 supercomputer, which in its first iteration will include 16 NVIDIA DGX H100 systems, each with eight NVIDIA H100 Tensor Core GPUs .

The DGX H100 is based on the powerful NVIDIA Hopper GPU architecture, which features a Transformer Engine designed to accelerate the training of transformer models , including generative AI models for biology and chemistry. Xeureka plans to add more nodes to the system as the project grows.

"Tokyo-1 is designed to address some of the barriers to implementing data-driven, AI-accelerated drug discovery in Japan," said Hiroki Makiguchi, product engineering manager in the science and technology division at Xeureka. "This initiative will uplevel the Japanese pharmaceutical industry with high performance computing and unlock the potential of generative AI to discover new therapies."

Customers will be able to access a dedicated server on the supercomputer, receive technical support from Xeureka and NVIDIA, and participate in workshops from the two companies. For larger training runs that require more computational resources, customers can request access to a server with more nodes. Users can also purchase Xeureka's software solutions for molecular dynamics, docking, quantum chemistry and free-energy perturbation calculations.

By using NVIDIA BioNeMo software on the Tokyo-1 supercomputer, researchers will be able to scale state-of-the-art AI models to millions and billions of parameters for applications including protein structure prediction, small molecule generation and pose prediction estimation.

Major Japanese pharma companies including Astellas Pharma, Daiichi-Sankyo and Ono Pharmaceutical are already making plans to advance their drug discovery projects with Tokyo-1.

Tokyo-based Astellas Pharma is pursuing innovative digital solutions across its business — including in sales, manufacturing, and research and development — to maximize outcomes for patients and reduce the costs of healthcare. With Tokyo-1, the company will accelerate its research with molecular simulations and large language models for generative AI through NVIDIA BioNeMo software.

"AI and large-scale simulations can be used for applications including small molecule compounds, antibodies, gene therapy, cell therapy, targeted protein degradation, engineered phage therapy and mRNA medicine," said Kazuhisa Tsunoyama, head of digital research solutions, advanced informatics and analytics at Astellas. "By enabling us to take full advantage of recent advances in AI and simulation technology, Tokyo-1 will be one of the foundations on which Astellas can achieve its VISION for the future of pharmaceutical research."

Tokyo-based Daiichi Sankyo will use Tokyo-1 to establish a drug discovery process that fully integrates AI and machine learning.

"By adopting AI and the cutting-edge GPU resources of Tokyo-1, we will be able to perform large-scale computations to accelerate our drug discovery efforts," said Takayuki Serizawa, senior researcher at Daiichi Sankyo. "These advancements will provide new value to patients by improving drug delivery and potentially enabling personalized medicine."

Ono Pharmaceutical, based in Osaka, focuses on drug discovery in the fields of oncology, immunology and neurology.

"Training AI models requires significant computational power, and we believe that the massive GPU resources of Tokyo-1 will solve this problem," said Hiromu Egashira, director of the Drug Discovery DX Office in the drug discovery technology department at Ono. "We envision our use of the DGX supercomputer to be very broad, including high-quality simulations, image analysis, video analysis and language models."

Beyond the pharmaceutical industry, Mitsui plans to make the Tokyo-1 supercomputer accessible to Japanese medical-device companies and startups — and to connect Tokyo-1 customers to AI solutions developed by global healthcare startups in the NVIDIA Inception program. NVIDIA will also connect Tokyo-1 users with the hundreds of global life science customers in its developer network.

Discover the latest in AI and healthcare at GTC , running online through Thursday, March 23. Registration is free.

Watch the GTC keynote address by NVIDIA founder and CEO Jensen Huang below:

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