

NVIDIA Opens BioNeMo to Scale Digital Biology for Global Biopharma and Scientific Industry

Argonne National Laboratory, Flagship Pioneering, Terray, Weights & Biases and Dozens More Organizations Among Contributors Advancing Biomolecular Science

SC24—NVIDIA today announced that global pharmaceutical and techbio industry leaders, academic pioneers and AI researchers are adopting the open-source [NVIDIA@ BioNeMo™ Framework](#) to advance drug discovery and accelerate molecule design.

Researchers require specialized biomolecular models and datasets that allow them to gather insights at scale to design therapeutics faster. The open-source BioNeMo Framework offers a collection of accelerated computing tools designed to exponentially scale AI models for biomolecular research, bringing a new level of supercomputing to biopharma.

“The convergence of AI, accelerated computing and expanding datasets offers unprecedented opportunities for the pharmaceutical industry, as evidenced by recent Nobel Prize wins in chemistry,” said Kimberly Powell, vice president of healthcare at NVIDIA. “To help unravel the complexities of biological systems, we’ve introduced the open-source BioNeMo Framework, which will enable researchers worldwide to accelerate the development of life-saving treatments.”

Pioneering biotech companies, techbio researchers and AI platform companies and organizations are already contributing or will contribute to the open-source framework, including A Alpha Bio; Argonne National Laboratory; Dyno Therapeutics; Genentech, a member of the Roche Group; Ginkgo Bioworks; Relation; VantAI and Weights & Biases. Key research leaders known for advancing computational science also use the BioNeMo Framework to drive innovation.

“Argonne has contributed billion-parameter biological models that require specialized software to train across high-performance computing environments,” said Arvind Ramanathan, computational science group leader at Argonne National Laboratory. “With BioNeMo, Argonne and the broader biotech community gain an enterprise-level, open-source solution that enables researchers to easily scale the training of large biological foundation models — in labs that otherwise wouldn’t have the computational expertise to do so.”

Introducing the Next-Generation BioNeMo Platform

The end-to-end [NVIDIA BioNeMo platform](#) is designed to accelerate AI model creation, customization and deployment for drug discovery and molecular design. Seamlessly integrated with accelerated computing infrastructure, it reduces costs, increases scale and speeds up drug discovery workflows to provide fast, reliable insights from biomolecular data.

In addition to the BioNeMo Framework, the platform supports [NVIDIA NIM™](#) — optimized microservices for secure, scalable AI inference — and NVIDIA BioNeMo Blueprints, which are optimized reference designs for wet-lab and computational workflows.

NVIDIA also announced a new collection of optimized, easy-to-use [NIM microservices](#) for BioNeMo. The microservices can be deployed quickly and easily on premises or in any data center or cloud. This offers developers the flexibility to run applications across a diverse range of environments and reduces the time from inference to insights for biological drug discovery research.

The newly available NIM microservices support industry-leading models, including:

- [AlphaFold2](#) is a deep learning model, developed by Google DeepMind, designed to transform protein structure prediction. Researchers using the AlphaFold2 NIM microservice for BioNeMo achieved a 5x speedup when predicting protein structures in near real time.
- [DiffDock 2.0](#) is based on MIT research and trained on the gold-standard [PLINDER dataset](#). With the DiffDock 2.0 NIM microservice, researchers were able to predict the orientation of a molecule 6.2x faster and 16% more accurately.
- [RFdiffusion](#) and [ProteinMPNN](#) NIM microservices help speed up the process of designing novel proteins to bind with a target molecule and enable the creation of new protein therapeutics.

BioNeMo now includes new acceleration libraries, including [cuEquivariance](#), that accelerate the mathematical computations essential to DiffDock predictions for chemistry.

Companies can use NVIDIA BioNeMo Blueprints, a catalog of customizable reference AI workflows, to help developers scale their AI deployments as enterprise-grade production pipelines.

The BioNeMo Blueprint for virtual screening provides a customizable, easy-to-follow workflow for using NIM microservices to design small molecules faster, while saving time and costs.

More than 200 techbios, large pharma and startup users are already integrating BioNeMo into their computer-aided drug discovery platforms and workflows.

Global system integrators, software providers and cloud service providers such as Accenture, AWS and Deloitte are bringing NVIDIA BioNeMo Blueprints to enterprises worldwide.

About NVIDIA

[NVIDIA](#) (NASDAQ: NVDA) is the world leader in accelerated computing.

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