

NVIDIA Partners with Schrödinger to Further Accelerate Drug Discovery Worldwide

Collaboration Enables Pharma Industry Giants, Biotech Startups to Use Schrödinger's Computational Drug Discovery Platform Boosted by NVIDIA DGX SuperPOD and NVIDIA Clara Discovery Libraries

GTC -- NVIDIA today announced a strategic partnership with Schrödinger that harnesses [NVIDIA DGX A100™](#) systems to further expand the speed and accuracy of Schrödinger's computational drug discovery platform and enable rapid, accurate evaluation of billions of molecules for potential development of therapeutics.

The companies will optimize [Schrödinger's](#) software platform — designed to model and predict the properties of novel molecules — for the [NVIDIA DGX SuperPOD™](#), which is built with NVIDIA DGX A100 systems and [NVIDIA InfiniBand HDR networking](#).

The work includes the physics-based modeling in Schrödinger's product suite, as well as support for [NVIDIA Clara™ Discovery](#), a collection of state-of-the-art AI frameworks, applications and pre-trained models for the most advanced computational drug discovery. Additionally, the companies will partner on scientific and research breakthroughs to further advance physics-based computing and machine learning for drug discovery.

For each potential drug candidate, Schrödinger routinely evaluates tens of thousands of molecules with its most computationally intensive physics-based approaches. This requires hundreds of thousands of hours of GPU time on high-performance computers.

Through the collaboration, the entire pharmaceutical industry comprising over 3,000 companies — from startups to multinationals — will be able to further accelerate drug discovery at supercomputing scale. The joint solution will enable companies of all sizes to simulate molecular combinations with physics and AI to identify and optimize the most promising compounds for potential therapeutic use. Pharmaceutical companies can run this research on their own easy-to-deploy private clouds featuring the Schrödinger platform running on [NVIDIA DGX SuperPOD](#), which is available to install on premises or in a colocation facility.

"The predictive modeling built into our platform is designed to dramatically expand and accelerate the search for high-quality therapeutic molecules, and NVIDIA is a key technology partner in this work," said Patrick Lorton, chief technology officer at Schrödinger. "Our advanced computational software helps the world's biggest pharma companies explore more of the chemical space and reach high-quality candidates more quickly, with far less compute cost, than traditional methods. We're proud to be working with NVIDIA to make that process run even more smoothly."

NVIDIA research and engineering teams are working to advance and optimize the Schrödinger suite to take advantage of the NVIDIA Ampere architecture and its [Multi-Instance GPU](#) technology. Customers will be able to easily deploy Schrödinger software on a single DGX system or a cluster of 20 or more to create a DGX SuperPOD. This allows scaling the Schrödinger platform to dozens of drug programs and screening and evaluating billions of molecules a week.

"Computational drug discovery is improving accuracy with Schrödinger's advanced combination of simulation with machine learning," said Kimberly Powell, vice president of healthcare at NVIDIA. "Together, we're giving the pharmaceutical industry a scientific instrument that delivers super-high-throughput lead generation to improve and accelerate the success of drug candidates."

About NVIDIA

[NVIDIA's](#) (NASDAQ: NVDA) invention of the GPU in 1999 sparked the growth of the PC gaming market and has redefined modern computer graphics, high performance computing and artificial intelligence. The company's pioneering work in accelerated computing and AI is reshaping trillion-dollar industries, such as transportation, healthcare and manufacturing, and fueling the growth of many others. More information at <https://nvidianews.nvidia.com/>.

Certain statements in this press release including, but not limited to, statements as to: the benefits and impact of NVIDIA and Schrödinger partnering and what it will enable; the companies optimizing Schrödinger's software platform; the benefits, impact and performance of our products and technologies; the companies advancing physics-based computing and machine learning for drug discovery; the work that goes into evaluating drug candidates; the collaboration enabling the pharmaceutical industry to accelerate drug discovery at scale and how they can use this technology; the availability of the Schrödinger platform; the benefits of predictive modeling built into the Schrödinger platform; Schrödinger's software helping the biggest companies; how NVIDIA is contributing to Schrödinger's work and advancing its suite of products; how customers can deploy Schrödinger software and what it allows; and how computational drug discovery is improving are forward-looking statements that are subject to risks and uncertainties that could cause results to be materially different than

expectations. Important factors that could cause actual results to differ materially include: global economic conditions; our reliance on third parties to manufacture, assemble, package and test our products; the impact of technological development and competition; development of new products and technologies or enhancements to our existing product and technologies; market acceptance of our products or our partners' products; design, manufacturing or software defects; changes in consumer preferences or demands; changes in industry standards and interfaces; unexpected loss of performance of our products or technologies when integrated into systems; as well as other factors detailed from time to time in the most recent reports NVIDIA files with the Securities and Exchange Commission, or SEC, including, but not limited to, its annual report on Form 10-K and quarterly reports on Form 10-Q. Copies of reports filed with the SEC are posted on the company's website and are available from NVIDIA without charge. These forward-looking statements are not guarantees of future performance and speak only as of the date hereof, and, except as required by law, NVIDIA disclaims any obligation to update these forward-looking statements to reflect future events or circumstances.

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