

## SHAPING THE FUTURE OF CRYO-EM WITH GPU<sub>s</sub>

How biomolecules function and interact is fundamental to understanding diseases, developing new drugs, and administering medical treatments.

Cryogenic electron microscopy (cryo-EM) is an imaging method that allows direct observation of proteins in native and near-native states without dyes or fixatives, giving researchers the ability to study cellular structures, viruses, and protein complexes in molecular detail.

This reconstruction of three-dimensional, near-atomic resolution structures of biomolecules often requires thousands of images and complex computing, making it difficult to deliver high-resolution structures.

Cryo-EM can help meet this challenge. Its success will be shaped by wider adoption, increasing data sizes, maturing of the market, and the rise of deep learning.

### MASSIVE DATASETS

The scope and complexity of cryo-EM data have greatly increased with advancements in automation and visual technology.

Cameras with higher sensitivity capture images at faster frame rates. With improved sample preparation, automation for data acquisition, and instrument uptimes, the requirements for data processing and computing continue to increase. For example, within a typical experiment, it often takes 1,000–8,000 images, captured from 4–8 terabytes (TBs) of raw image data, to generate high-resolution, single-particle maps.

Over the past few years, almost all compute-intensive steps in single-particle workflows have been ported to take advantage of GPU processors, which shorten processing times dramatically. To keep up with increasing data sizes, cryo-EM applications need to be optimized for higher-end GPUs.

### THE MATURING MARKET

Traditionally, processing cryo-EM image data to uncover protein structures and create high-resolution 3D maps requires expert intervention, prior structural knowledge, and weeks of calculations on expensive computer clusters.

As it becomes mainstream, cryo-EM is fostering demand for commercial-grade, non-expert software. These software solutions involve using algorithms to automate specialized and time-intensive tasks.

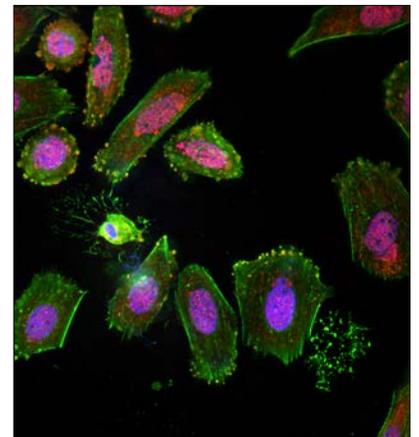


Image credit: Microvolution

Within Merck's structure-based drug-design pipeline, for example, they use the cryoSPARC software suite. The cryoSPARC platform uses NVIDIA GPUs to enable automated, high-quality, and high-throughput structure discovery of proteins, viruses, and molecular complexes for research and drug discovery.

## INFUSION OF DEEP LEARNING

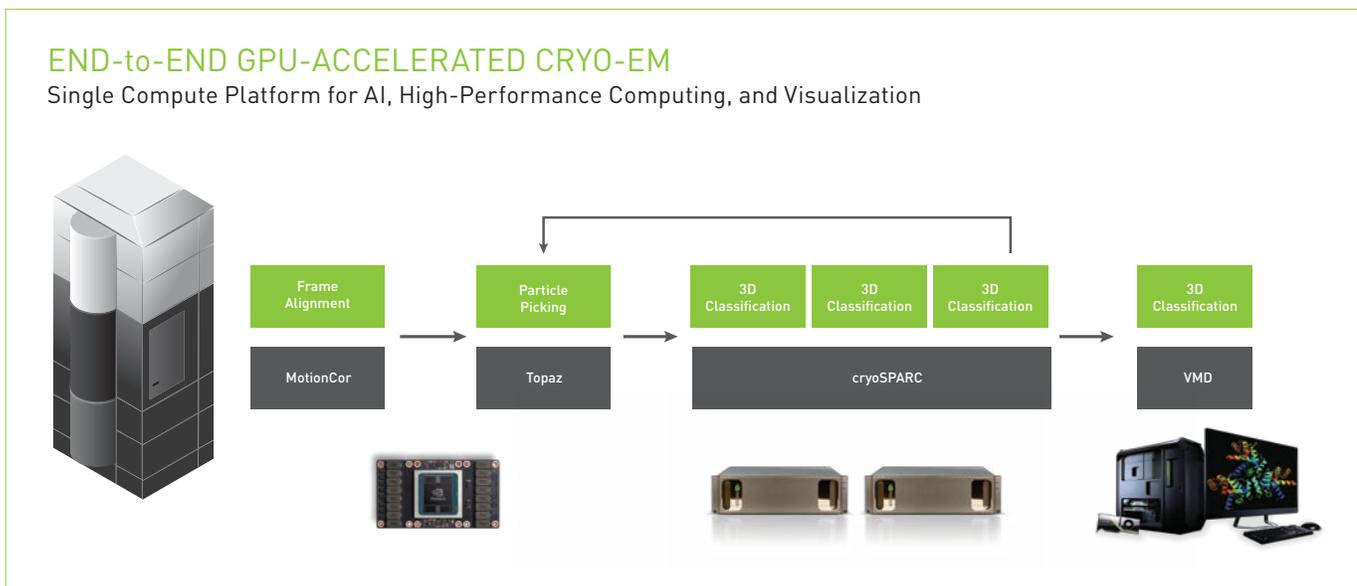
Selecting individual protein particles in cryo-EM micrographs is an important step in the single-particle analysis. It's challenging to identify the particles due to a low signal-to-noise ratio and the tremendous variations that occur in biological macromolecular complexes.

By leveraging positive-unlabeled learning, a small number of example protein projections can train a neural network to detect proteins of any size or shape. Topaz, an open-source application with this capability, detects significantly more particles than other software methods when tested. Powered by NVIDIA GPUs, it drastically cuts down the amount of data that needs to be manually labeled.

## GPUs IN THE CRYO-EM WORKFLOW

Cryo-EM methods are opening up opportunities to explore the complexity of macromolecular structures in previously inconceivable ways. From early-phase research systems to large data centers, GPUs are enabling end-to-end workflow acceleration. By optimizing key workloads for data acquisition and single-particle reconstruction, GPUs continue to deliver paths to scientific and healthcare breakthroughs.

With GPU-based computing and deep learning, advancements in cryo-EM will increase its reliability and output and, ultimately, its adoption and success.



Learn more about [NVIDIA in cryo-EM](#).