Accelerate drug discovery with Rescale on AWS and NVIDIA

In collaboration with:

rescale

High performance computing (HPC) helps researchers and computational scientists expedite early stage research and speed up drug development

$4 billion

average cost of developing a new drug and making it available for treatments[1]

21.7%

of revenue spend on R&D in healthcare and pharmaceuticals industries[2]

The process of finding the right drug candidate suitable for preclinical and clinical trials is like searching the beach for one perfect grain of sand. Out of hundreds of thousands of compounds screened and analyzed for various characteristics, only one or two make it to clinical trials. Of that, only about 10-12 percent[3] reach the market—and that's after years and billions of dollars spent on clinical research.

Computer-aided drug design (CADD), high-throughput screening (HTS), and AI-based drug discovery tools help speed up early research, allowing scientists to sift through compounds faster. However, outdated infrastructures and massive, siloed datasets prevent researchers from using these tools to their full potential.

Challenges facing early research and clinical trials

Data is the solution. And the problem.

The biopharmaceutical industry has been generating more data than ever. All this data presents an incredible opportunity to uncover deeper insights and find solutions to even the most complex clinical cases. The challenge lies in harnessing its potential.

Pharmaceutical companies must generate, manage, and analyze increasingly vast quantities of data efficiently and effectively. Collaboration is critical and security is non-negotiable. Above all, researchers must generate high-quality data and trusted insights. From drug design and polypharmacology, to drug repurposing and screening, cutting-edge analysis underpins clinical breakthroughs, speed to treatment utilization, and financial viability[4].

It's hard to imagine achieving a data-driven competitive advantage without HPC. And for most drug discovery workloads, it's hard to imagine HPC without the cloud.

Clinical trials rightly remain the benchmark for any new drug. However, enrolling and engaging participants is typically time-consuming and expensive (and sometimes ethically problematic.)

HPC-powered analysis and artificial intelligence (AI) simulations rapidly narrow the field of potential drug candidates and new applications for existing compounds—dramatically reducing the required number of trials and their associated costs and logistical considerations.

The ability to simulate multiple models before real clinical trials, such as Pharmacokinetic-Pharmacodynamic (PKPD) Analysis, is undeniably powerful. It also demands daunting amounts of computational power.

In-house infrastructure typically falls short, due to the spikey nature of research workloads, increasing computational requirements, and budget overruns. Fortunately, leveraging HPC in the cloud with Amazon Web Services (AWS) makes it possible for pharmaceutical companies to rapidly scale even the most computationally demanding stochastic modeling and simulation workloads with elastic resources and a pay-as-you-go approach.

With that in mind, let's explore common hurdles in the early research and clinical trial phases of drug discovery.

Early research

The more simulations pharmaceutical companies can run, the faster they can identify promising compounds or innovative applications and progress to clinical trials. However, early research is impeded by the following challenges, all of which underscore the need for efficient, scalable, and cost-effective HPC resources.

Declining R&D productivity

The average expected return on investment (ROI) for global research and development fell from 6.8 percent in 2021 to 1.2 percent in 2022 according to a Deloitte analysis of 20 leading pharmaceutical companies[5]. The analysis goes on to show R&D is taking longer and costing more than it did 10 years ago.

Silos and bottlenecks

Researchers may store data in multiple locations—on separate spreadsheets, an internal server, or with an external partner. All these locations likely have different practices and naming conventions, making data difficult to find, organize, and use. The process becomes even more complicated when adding different data modalities, like medical imaging and genomics.

Budget constraints

AI-enabled drug discovery platforms promise efficiency gains for research teams. However, publicly available methods may not meet business needs and building tools in-house is both complex and costly. Larger pharma companies may choose this route for intellectual property and customization reasons, but development could drag on for years.

Aging infrastructure

Legacy on-premises servers lack the capacity and reliability to handle the HPC and GPU-powered AI used in today's drug discovery workloads. As rack densities increase to attempt to manage the load, so do the costs required to cool and maintain the equipment.

Clinical trials

Scientists use a variety of medicinal chemistry and drug design strategies to find molecular entities with the potential to progress to clinical trials.

Advanced assay and screening technologies allow scientists to evaluate more compounds faster. AI is being used to predict drug-protein interactions and drug efficacy[6], among other applications.

CADD involves compute-intensive digital simulations that require HPC parallelized clusters. Organizations that use hundreds of applications may require multiple computing architectures to power these massive workloads. While CADD allows scientists to find drug targets faster and more cost-effectively than laboratory testing, many research organizations are limited by their infrastructure.

Limited HPC resources

The demand for HPC resources within a company can have substantial peaks and troughs based on the drug design or discovery stage and the amount of simulation work needed on a given day or week. The peaks may expand beyond the capacity of an on-premises data center, requiring complex job scheduling and prioritization to minimize bottlenecks and delays.

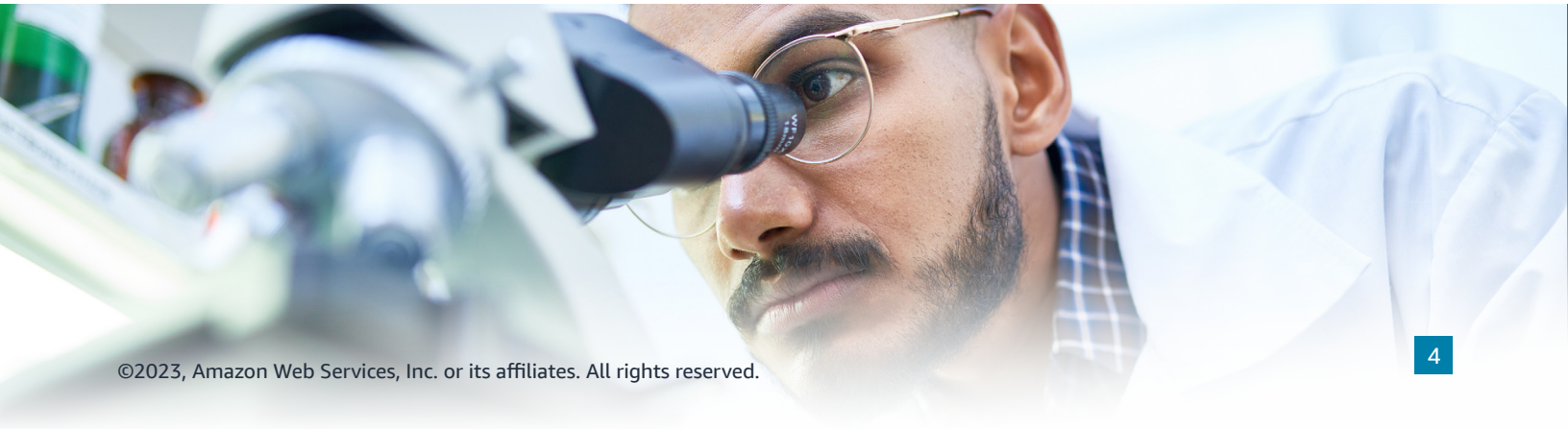
Moreover, it's not financially feasible to build an on-premises data center to accommodate peak capacity, because the trough periods would not justify the expense. The same reasoning would apply to installing a wide range of computing architectures optimized for each individual application.

Queued jobs

Limited infrastructure means computational scientists may have to wait days to weeks while simulation jobs are queued in the on-premises HPC system. It is also difficult for on-premises HPC data centers to have multiple hardware architectures to support a variety of software types. Without matching the right hardware to application needs, simulations can run slower than optimal.

Management burdens

HPC software for drug research requires constant updates and maintenance to ensure complex simulations run dependably. Scientists don't want to waste time installing and maintaining software. Nor should they. They need to devote their time to what they do best—pioneer new life-saving drugs.



Running HPC, AI/ML-powered workloads on Rescale

The right molecules are out there, somewhere. Researchers just need the tools to find, develop, and trial them faster and more cost-effectively. That means it's time to rethink the traditional in-house infrastructure model.

With Rescale as the foundation, working with AWS and NVIDIA, computational scientists benefit from an HPC solution that's user-friendly, agile, and fast.

NVIDIA provides hardware and GPU-accelerated software for life sciences workloads. It offers the latest enterprise-grade AI frameworks and optimized GPU simulation application containers that run in the cloud. It also provides latest instances to speed-up life science simulation applications and AI framework performance while maximizing overall data center efficiency. AWS offers elastic, high performance on-demand access to the latest architectures from NVIDIA at the scale needed to run complex life science applications. With the most extensive, most secure global infrastructure, AWS offers massive scale potential so you can quickly and easily scale to meet the highest demand and seamlessly scale down to reduce costs. As the largest cloud provider with hundreds of integrated features and services, AWS offers a wide range of specialized hardware architectures, making it an ideal complement to NVIDIA.

When deploying HPC and AI in the cloud, computational scientists can build and orchestrate more efficient R&D studies with flexibility to harness the latest, best-fit hardware and software on-demand at virtually unlimited scale.

High performance computing 'built for the cloud' empowers scientists while delivering IT security & control

Traditional HPC (on-premises or cloud)

Hardware-centric – Focused on HW utilization
Inflexible – Predefined HW, SW and fixed capacity
Siloed – Isolated islands of analysis
Static – One-time tuning with stagnant configs
Manual – Script-based, complex operations

Constrained scientific innovation, inefficient use of talent & resources

HPC built for the cloud

User-centric – Intuitive with SaaS-like simplicity
Unlimited – Any scale, any architecture, any application
Connected – Seamless, secure, global collaboration
Intelligent – Continuous performance optimization
Automated – Policy-driven control and end-to-end workflows

Accelerated R&D initiatives, new possibilities

Rescale HPC platform

The Rescale platform provides HPC-as-a-service that makes deploying a full-stack HPC environment for modern life sciences research fast and simple.

With it, computational scientists can instantly access:

- A catalog of pre-installed life sciences simulation applications
- The latest optimized hardware architectures for application performance
- NVIDIA frameworks for custom/in-house and open-source AI/ML workflows
- Optimized GPU simulation application containers running on Amazon EC2 instances powered by NVIDIA GPUs
- Secure data sharing and collaboration across teams

With the Rescale platform, you have all the compute power and software needed as a foundation to AI-driven drug discovery.

“Rescale automates cloud HPC complexity, making job submission as easy as a few clicks”

See how Rescale can scale your computing capabilities ›

Accelerate drug discovery with Rescale

Easy to use interface

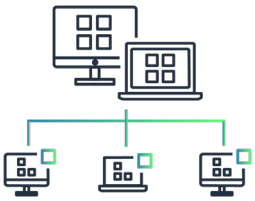
Rescale offers powerful HPC in a simple, user-centric experience to accelerate your next drug development breakthrough. Get started faster with fewer steps and focus on pharmaceutical innovation without complexity. Flexibly interact with simulations through Rescale's automated graphical user interface (GUI), command line interface, or API.

HPC software catalog

Run any application for early research and clinical trials. Access 1000+ pre-installed commercial, open-source, and custom HPC and AI/ML software, including the latest and previous versions. No maintenance or updating required. Rescale includes on-demand licensing, with hosting and queuing to maximize your existing licensing. Benefit from the support of Rescale experts to help you run your most demanding workloads.

Specialized hardware catalog

Get the best performance for your drug discovery workloads with the largest selection of architectures in the cloud. Choose from a variety of the latest specialized HPC and AI hardware, including CPUs and GPUs. On-demand and pre-tuned for performance, Rescale Coretypes deliver results faster, based on your requirements for clock-speed, memory, interconnect, and storage.



Enhanced infrastructure

Utilize the agility and elasticity of AWS with confidence. Get more from your cloud spend with Rescale's job-level guarantees for job start and completion to ensure business continuity and eliminate failed jobs while prioritizing performance, efficiency, and cost model flexibility for each workload.

Full-stack security

Pursue clinical innovation while ensuring strict compliance with data security and privacy regulations. Rescale security standards include: FedRAMP Authorized (moderate), ISO 27001, SOC 2 Type 2, ITAR, HIPAA, CSA Registered, TISAX Level 1, GDPR, and CCPA. Rescale follows the NIST 800-53 framework to provide zero trust security architecture complementing AWS' underlying security principles and advanced capabilities for end-to-end security models for environments built on top of AWS services.

Integrated file management

Unify data with workloads in the cloud and reach greater productivity, collaboration, and efficiency by organizing data by jobs or by file attributes. Manage storage costs and job integrity with policy-driven retention and deletion of files, jobs, and directories. Seamlessly connect data sources to deliver secure and controlled access at the organization, project, and user levels.

Performance Profiles

Rescale automates manual application benchmarking practices, so your R&D scientists and researchers can keep up with the rapidly expanding choices in specialized chips and cloud services. Easily determine cost, performance, and carbon footprint of your workloads across each application.

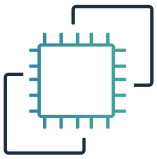
Optimized performance powered by AWS and NVIDIA

NVIDIA Clara for Drug Discovery

Benefit from a collection of GPU-accelerated and optimized frameworks, applications, generative AI platforms and pre-trained models for AI drug discovery pipelines. Built to support cross-disciplinary workflows, Clara for Drug Discovery helps computational biologists, computational chemists, and AI drug discovery researchers understand disease mechanisms to get drugs to market faster.

NVIDIA NGC suite

Take advantage of a variety of services, software, and support for AI, digital twins, and HPC. This suite includes GPU-accelerated frameworks such as PyTorch, an optimized tensor library for deep learning. Applications such as GROMACS and LAMMPS allow scientists to test molecular dynamics and simulation applications. These and other tools help scientists explore structure and function of proteins and molecules, accelerating lead generation.



Amazon Elastic Compute Cloud (Amazon EC2)

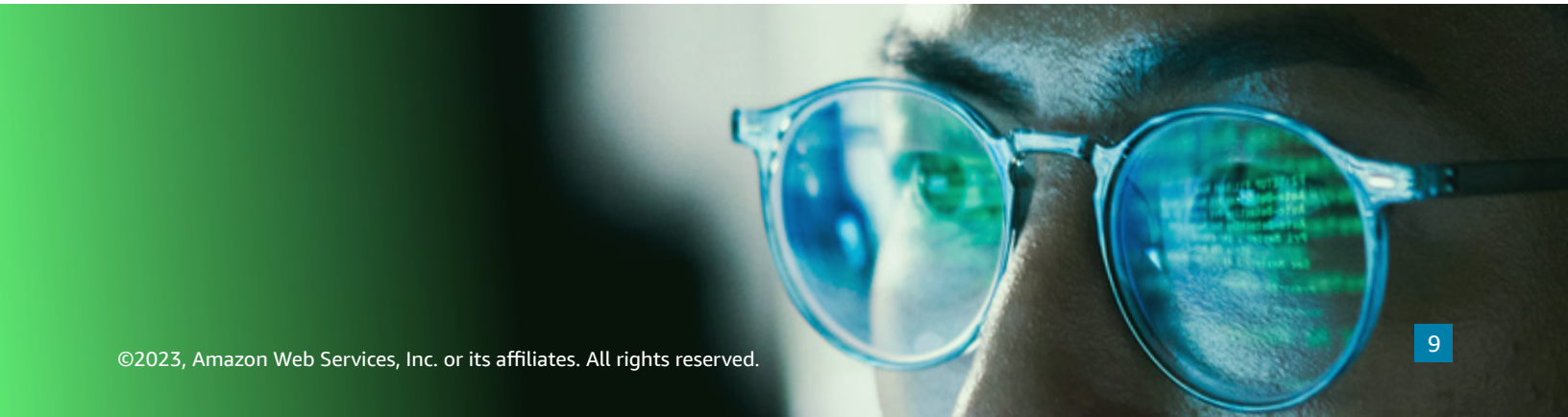
Amazon EC2 provides reliable compute capacity for the most data-intensive and demanding HPC workloads. Amazon EC2 works with NVIDIA and Rescale to facilitate computationally demanding tasks such as molecular modeling, deep learning, and next-generation sequencing.

When paired with NVIDIA on Rescale, computational scientists significantly reduce time to results while reducing infrastructure costs.

Amazon Simple Storage Service (Amazon S3)

Amazon S3 provides secure, scalable data storage for molecular research and simulations.

This powerful service ensures a consistent user experience among teams spread across the globe.



Why Rescale

Rescale makes using cutting-edge NVIDIA GPUs and software on AWS "push-button easy." Scientists can run simulation applications or AI-based tools on AWS, powered by NVIDIA GPU-accelerated Amazon EC2 instances without calling upon IT support.

Rescale aligns with existing IT policies to ensure strict regulatory compliance. It also allows scientists to produce accurate data and simulation history for review by the FDA and other regulatory bodies.

As a cloud-based platform, Rescale scales with your project. Research teams can adjust computational resources based on the complexity and urgency of the tasks at hand. This ensures continuous performance optimization and cost efficiency.

With Rescale's built-for-the-cloud HPC platform, researchers can run workloads of any system type—including bare metal, virtualized, or container-based on the cloud infrastructure of their choice. The platform runs fully virtualized on AWS.

Rescale's industry-leading compliance standards

Rescale, AWS and NVIDIA together

AWS offers reliable cloud computing services that scale elastically according to research needs, while NVIDIA provides GPU technology optimized for scientific computing and AI to accelerate simulations and calculations. Rescale offers a secure platform for running simulations and models accelerated by AWS powered by NVIDIA GPUs and stored on the AWS cloud. End result: Go fast, deploy faster, without limitations.

Access to enhanced simulation capabilities and screening work in a scalable and pay-as-you-go workflow on the Rescale platform is enhanced by AWS services powered by NVIDIA technology.

Because Rescale uses AWS and NVIDIA technology it enables research teams to access advanced collaboration and data transfer tools. Teams can share jobs to better allocate resources among various projects and teams, leading to significant cost savings.

And with research data stored in the AWS cloud, teams can more easily integrate data sources, dramatically reducing repetitive manual tasks.

Drug discovery in the cloud

Scientific and technological advances have moved drug discovery from a solely physical discipline to both physical and virtual. Data-intensive processes such as AI and computer-aided drug design stress legacy infrastructures. By migrating workloads to a cloud-based framework built with AWS, NVIDIA, and Rescale, research teams have the capacity they need to accelerate drug discovery in a cost-effective manner, paving the way to improved ROI and quicker development of life-saving drugs.

Innovative drug discovery use cases powered by HPC and AI/ML

New drug development
Integrating machine-learning techniques to create new molecules.

Emulating biological processes
Applying regression-based transfer learning to model responses to anticancer medication.

Drug development and testing
Using genetic and medicinal data to monitor the signals between the pathways where the molecules of the drug traveled.

Drug–target interaction
Combining multiple machine learning (ML) algorithms and sub-categories to analyze and monitor how drugs interact with their targets.

Post-manufacture drug reviews
Harnessing multitask learning and analysis algorithms to analyze data in bulk.

Accelerate key applications

Drug discovery spans many specialized use cases, from exploring the chemical universe and predicting protein structures to scanning drug candidates and simulating molecules. The Rescale platform includes several applications to facilitate these complex workflows, including:

GROMACS
Used to simulate molecular dynamics (MD), primarily for biochemical molecules

NAMD
A parallel MD code designed for high performance simulation of large biomolecular systems

VASP
A popular program for atomic scale materials modeling, used to perform ab initio quantum mechanical calculations

Quantum Espresso
An integrated suite of open-source computer codes for electronic-structure calculations and materials modeling at the nanoscale

Siesta
A method and its computer program implementation (Fortran 95) to perform efficient electronic structure calculations and ab initio MD simulations of molecules and solids

Case study: How a lean biotech start-up accelerated genome and peptide discovery research from five days to 24 hours

"As a researcher, I don't have much experience in IT, so I was nervous migrating our HPC to the cloud. But Rescale's user-friendly platform did not require expertise in IT or HPC. Also, Rescale understands both HPC and R&D fields, which provides us crucial support and lets us focus solely on R&D."

Dr. Hyejin Park, Director, AI Research Institute, AZothBio

Challenge: AZothBio, a biotech company based in Seoul, Korea, uses digital tools and proprietary AI logic to uncover new drug and therapy candidates. When its compute demands exceeded the capabilities of their on-premises hardware, leadership knew the company needed a scalable cloud-based alternative. They not only wanted capacity but also more agility for the R&D team.

Solution: AZothBio partnered with Rescale and AWS to run their workloads. The company created a more efficient, cost-effective research system for selecting drug candidates. It also accelerated lead identification through massive data analysis and predictive simulation using their own proprietary deep learning-based algorithms in ways not possible with their on-premises HPC computers.

Results: Through Rescale, the team gained access to pre-installed software and the best-fit GPU hardware to successfully run their epitope AI models. Most importantly, the biotech company was able to reduce its genome and peptide discovery research from five days to within 24 hours per analysis.

Accelerate your drug discovery workloads today with Rescale on AWS, powered by NVIDIA ›

[1] "What Are the Average Research and Development Costs for Pharmaceutical Companies?," Investopedia, 2022
[2] "What Are the Average Research and Development Costs for Pharmaceutical Companies?," Investopedia, 2022
[3] "Research and Development in the Pharmaceutical Industry," Congressional Budget Office, 2021
[4] "Artificial intelligence and machine learning in drug discovery and development," Science Direct, 2022
[5] "Deloitte pharma study: Drop-off in returns on R&D investments – sharp decline in peak sales per asset," Deloitte, 2023
[6] "Machine Learning in Drug Discovery: A Review," National Library of Medicine, 2021