

Bringing the power of high-performance computing to drug discovery and healthcare

How Oracle Cloud Infrastructure is helping organisations accelerate drug discovery and modernise healthcare

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Summary

While the underlying drivers of the pharmaceutical (pharma) industry, such as an aging population, prevalence of chronic conditions, demand for treatments of rare conditions, and emerging novel viruses, remain strong, the industry is under pressure to change. A core focus for industry transformation is addressing drug development cost structures and improving development effectiveness. Not only are current processes lengthy and costly (typically 10 years at a cost of US\$2.5 billion to bring one therapy to market¹), but the ability to produce “blockbuster” therapies that compensate organisations sufficiently to cover these massive efforts is now a top priority. A blockbuster therapy generates annual sales of at least US\$1 billion for the company that sells it.

Improving research and development (R&D) productivity is contingent—to a large extent—on the ability of organisations to collect, organise, analyse, and interpret data from a wide array of sources beyond traditional clinical studies. While the value, variety, volume, and veracity of such data is increasing rapidly, organisations are still struggling to keep pace using conventional data-management approaches. However, the speed at which organisations can discover and develop more-ambitious therapies is increasingly important in achieving competitive advantage, as being first to the market is key.

The time it takes to get a therapy to market can be shortened—even by several years—by leveraging innovative, cloud-based technologies to accelerate drug discovery and therapeutic development. Cloud technology is changing what is possible, especially in data-driven, computationally intensive R&D processes. Moreover, research projects need secure, robust, reliable, and scalable infrastructure that can be provisioned quickly. Oracle’s technologies in high-performance computing (HPC), advanced analytics, artificial intelligence (AI), and machine learning are core components in transforming the economics of pharmaceutical R&D productivity.

As unlike first generation cloud vendors, Oracle Gen 2 Cloud has been architected for security, performance/price and comprehensive end-to-end SLAs covering performance, availability, manageability of services.

For example, researchers at Flinders University and University of Bristol turned to Oracle for Research, which supported them and their teams with a one-year Oracle for Research grant, providing access to Oracle Cloud Infrastructure and technical advising and collaboration. Flinders University

“We processed the large data sets obtained by the microscope on the cloud in a fraction of the time and at much lower cost than previously possible. We took a 90-day process and completed it in under five days with Oracle Cloud HPC.”

Christopher Woods
EPSRC Research Software
Engineer Fellowship

¹ European Federation of Pharmaceutical Industries (2013): Estimated full cost of bringing a new chemical or biological entity to market

have designed a novel COVID-19 vaccine candidate. The research team analysed computer models of the SARS-CoV-2 spike protein and its human receptor ACE2 to identify how the COVID-19 virus infects human cells at a pace that was dramatically increased². In another example, the University of Bristol recently discovered a synthetic vaccine to the mosquito-borne chikungunya virus in a fraction of the time and at a much lower cost than previously thought possible, leveraging on-demand access to a large number of Oracle Cloud Infrastructure processors³ to perform large scale simulation.

High-throughput screening for top-10, global pharma company

Oracle for Research is a global community that is working to address complex problems and drive meaningful change in the world. The program provides scientists, researchers, and university innovators with high-value, cost-effective Cloud technologies, participation in Oracle research user community, and access to Oracle's technical support network. Through the program's free cloud credits, users can leverage Oracle's proven technology and infrastructure while keeping research-developed IP private and secure. Unlock your research possibilities.

[Learn more](#)

Rethinking the pharma industry business model

With the emergence of new diseases and the prevalence of hard-to-cure diseases, pharma organisations continue their relentless pursuit to discover new drugs. The average time from drug discovery to regulatory approval is approximately 10 years, and only one out of approximately 5,000 possible candidate drugs is approved. These data points indicate the high-stakes play involved in discovery of new therapeutic drugs. It could take between three-to-five years to discover new candidate drugs that are passed on to the preclinical stage.

Pharma organisations are examining R&D cost structures in the face of intensifying demand and directives to save money. On the demand side, the traditional revenue model is under pressure, as patents of blockbuster drugs expire, and the likelihood of creating additional blockbuster drugs diminishes. Furthermore, there is increased competition from generics, biosimilars, and thin drug therapies with added pressure from reimbursement models and pricing.

On the cost side, there is the manifestation of Eroom's law. Eroom's law is the observation that drug discovery is becoming slower and more expensive over time, despite advances in science and technology. If this trend continues, the expenses for a newly approved drug will reach unprecedented values over the next few years.

A core tenet to fundamentally changing the economics of drug development is the adoption of innovative technologies to accelerate and expand drug discovery and development pipeline. Cloud-based technologies have not only matured significantly over recent years, they are now indispensable in

² Flinders University (2020): *Flinders targets COVID-19 vaccine*

³ PROFIT (2019): */increasingly, researchers are moving their specialized workloads to the high-performance cloud*

exploiting data more effectively, helping pharma companies remain competitive in this quickly changing industry.

Precision medicine and Big data

Precision medicine centres on the possibilities of testing patients for certain biomarkers and matching them to more individualised and appropriate treatments. The approach targets therapies to a subgroup of patients, instead of the traditional one-drug-its-all model. The discipline has advanced rapidly in recent times, leveraging bioinformatics and related techniques to assist clinicians in gathering and interpreting big data. Although individual, niche therapies may fall short of conventional blockbuster status, there is potential for such drugs to target a range of niche segments to achieve a 'new' blockbuster status.

Successful adoption of precision medicine for diagnosis, determining drug efficacy, and treatment response is not free of problems.

Important consideration needs to be given to storage, backup, analysis, and interpretation of data, protecting the privacy of the patient, ensuring data security, and limiting human errors while handling data. Sources of data include electronic medical records (EMRs), genetic profiles, wearables, and connected devices. The value, variety, volume, and veracity of data that needs to be processed is increasing rapidly; however, organisations are struggling to effectively manage and handle that data with conventional data-management approaches.

Accelerating drug discovery with HPC and AI

Cloud-based technologies, such as HPC and AI, are increasingly being used by pharma organisations to probe vast amounts of raw human biological data to discover new insights into complex clinical causes of human disease and new opportunities for diagnosis and treatment.

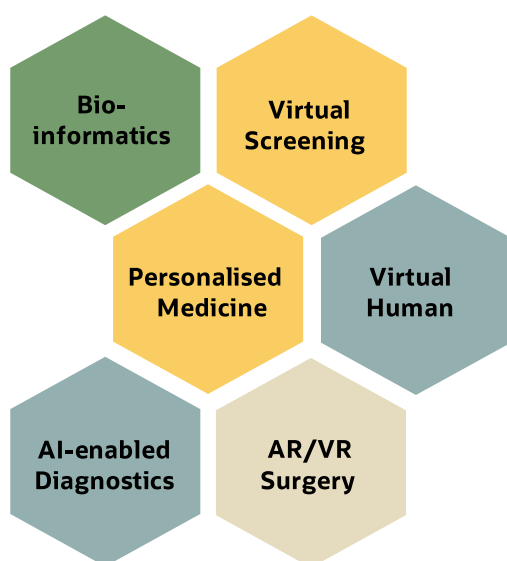
Furthermore, the complexity of R&D processes often requires collaboration between multiple, global sites, with contract research organisations (CROs), or through partnerships with other pharma or academic institutions. This involves data collection, storage, transmittance, management, analysis, and interpretation.

These complex projects need to ensure that the data is secure, safe, and handled with a robust, reliable, and scalable infrastructure. Moreover, they need the ability to easily provision technology, analyse complex information, and output results in a desirable format for downstream applications.

CORE PHARMA CHALLENGES	CLOUD HPC VALUE	EXAMPLE OUTCOMES
<ul style="list-style-type: none"> Accelerate drug discovery and the treatment development process Rapidly analyse and interpret data streams derived from clinical studies Identify new therapies for disease sufferers not served by standard treatments Match the right treatment(s) to the right patients more effectively 	<ul style="list-style-type: none"> Enable analysis of larger quantities of data from clinical studies, DNA, genetic testing, and EMRs, facilitating discoveries not previously possible Reverse engineer data-driven models of human disease progression and drug responses Simulate models to discover novel drug targets Automate components of the end- to-end R&D process Gain the ability to increase capacity to meet spikes in activity and reduce waiting times Pay for resources consumed only as they are consumed 	<ul style="list-style-type: none"> Drive faster time to value, and reduce time needed to conduct complex network analysis from months to weeks Conceive more-ambitious projects not conceivable before cloud-based HPC, and ask 'bigger' questions Support effective and productive partner collaborations to facilitate quicker outcomes Put control directly in the hands of the research teams that consume HPC infrastructure Focus on strategic priorities and HPC outcomes, rather than managing infrastructure or fighting for capital budget on new hardware Save on cost, which can contribute to more-competitive pricing

Sample use cases in drug discovery and healthcare

Early adopters of Cloud HPC and AI in the industry have already demonstrated its potential to transform scientific discovery. The applicability and value of these technologies stems across the Pharma value chain.



Bioinformatics

Bioinformatics involves application of computational theories and algorithms for analysis of biological data. This is a multidisciplinary field, which requires knowledge of biological sciences, mathematics, information science, computer science, and statistics.

Genomic sequencing is one of the most-important HPC use cases under the bioinformatics umbrella. During the past few decades, significant growth in available computing power has made challenging sequencing problems, such as whole genome sequencing (WGS), computationally feasible and financially viable. HPC plays an important role in making WGS feasible, and fuels advances in high-through- put or next-generation sequencing (NGS).

With NGS it becomes possible to analyse millions of genomic sequences in a single run. Cloud HPC provides the flexibility to scale up resources and drastically reduce the time taken to analyse genomic sequence data. Oracle Cloud Infrastructure supports genomic sequencing libraries, such as, NVIDIA Clara Parabricks, which take advantage of NVIDIA's latest-generation graphics processors to reduce time to results.

Virtual screening

Computational chemistry is a discipline that utilises molecular-level information from the biological target sites related to a disease, such as proteins or enzymes, to find the chemical compounds with the potential for treating the health condition. Computer-aided identification of potential drug molecules involves a process called virtual screening. A combination of virtual screening and a computational technique called molecular dynamics simulation helps in narrowing down the number of candidate drugs from tens of thousands to hundreds. The computer-aided drug discovery process can be significantly accelerated by using Oracle Cloud Infrastructure HPC.

Personalised medicine

Personalised medicine identifies the most suitable treatment plan for a patient based upon genetic information. An example of precision medicine is seen in cancer treatment where the genomic sequence of tumour cells is used in identifying the mutation that was responsible for the disease. Identification of a particular mutation in genomic sequence helps in pinpointing the most-effective therapeutic regime for treating the disease. The flexibility to scale up sequencing analysis on Oracle Cloud Infrastructure HPC can help identify the best treatment plan in less time and improve clinical outcomes through wider adoption of precision medicine.

Virtual human

Designing medical devices, such as heart valves, stents, and pacemakers, requires careful consideration of the human body's interior structure. When it comes to implanting a device inside a vital organ, there is no room for error. Imaging modalities, such as, X-rays, MRIs, and CT scans, provide two-dimensional images of internal organs.

A composite model can be created using these images, which provides a three-dimensional, virtual representation of the human body. This virtual

human provides the flexibility to conduct infinite trials of a medical device before implanting it inside the body. Measuring the effectiveness of devices is accelerated by running simulations on the thousands of CPUs that reside in a cloud HPC cluster.

AI-enabled diagnostics

AI algorithms for computer vision can process images to identify diseases with high precision, making the work of clinicians easier. It is possible to implement these AI systems on a large scale by leveraging Oracle Cloud Infrastructure HPC. Beyond the diagnostic applications, AI algorithms can also be used in drug discovery where generative algorithms help in designing new drug molecules that have potential to provide a cure for hard-to-treat diseases.

Augmented reality/virtual reality surgery

All surgical procedures carry the risk of an adverse outcome—especially cardiovascular and neurological surgeries. Advances in virtual reality (VR) technology allow surgeons to rehearse their surgical plan on a realistic, virtual patient model before entering the operating room to minimise the risks associated with surgery. Oracle Cloud Infrastructure HPC enables medical professionals to explore complex structures in a VR environment. Excellent use of CPU/GPU resources and state-of-the-art networking help in rendering the VR scenes without any glitches or delays, providing a realistic experience.

Case study 1—Acceleration of powerful vaccine discoveries

University of Bristol

Challenge:

Stop the spread of the infectious, mosquito-borne disease chikungunya that was spreading throughout the world at an alarming pace. Traditional vaccine design and production technology resources impeded innovative vaccine discoveries.

Approach:

Design a novel vaccine delivery system that is easy to produce in high volumes.

Use the company's on-premise supercomputers and leverage the power of cloud HPC to process very large data sets from the cryo-electron microscope, which is integral to digital modelling for their pioneering vaccine research.

Output:

Developed a novel, computational approach using Oracle Cloud Infrastructure HPC to create an accurate, high-resolution digital model of their synthetic vaccine in a fraction of the time and at a much lower cost than previously thought possible.

Envisaged a vaccine delivery system from a lab-produced, thermostable, protein molecule that could be readily manufactured at low cost and does not require refrigeration to retain viability.

Case study 2—High-throughput screening of potential candidate molecules

Top 10 Pharma Co.

Challenge:

Improve screening throughput of its potential candidate molecules. The company was achieving one million molecules in about 24 hours using their in-house HPC cluster.

Approach:

Create a proof of concept to run the pharma company's open source-based screening process through HPC on Oracle Cloud Infrastructure as a comparison to their in-house HPC cluster.

Core Oracle solutions include Oracle HPC (VM and bare metal), Oracle Cloud Infrastructure Object Storage, and Oracle Cloud Infrastructure Container Engine for Kubernetes running Redis Database and SLURM Workload Manager.

Output:

Oracle was able to improve screening productivity from one million molecules in 24 hours to one million molecules in seven minutes and 25 seconds (at a cost of US\$48).

NVIDIA Parabricks available on Oracle Cloud Infrastructure, which can cut analysis time from 30 hours to just under one hour.

Oracle's heritage in health sciences and emerging technologies

Oracle has been serving the health sciences industry with emerging technologies for nearly 40 years. Oracle's comprehensive solutions for health sciences help address the ever-increasing need to collect, manage, analyse, and collaborate on data. These technologies help researchers spend less time building, deploying, maintaining, analysing, and securing IT, and more time interpreting, discovering, and collaborating.

Oracle Cloud Infrastructure Generation 2

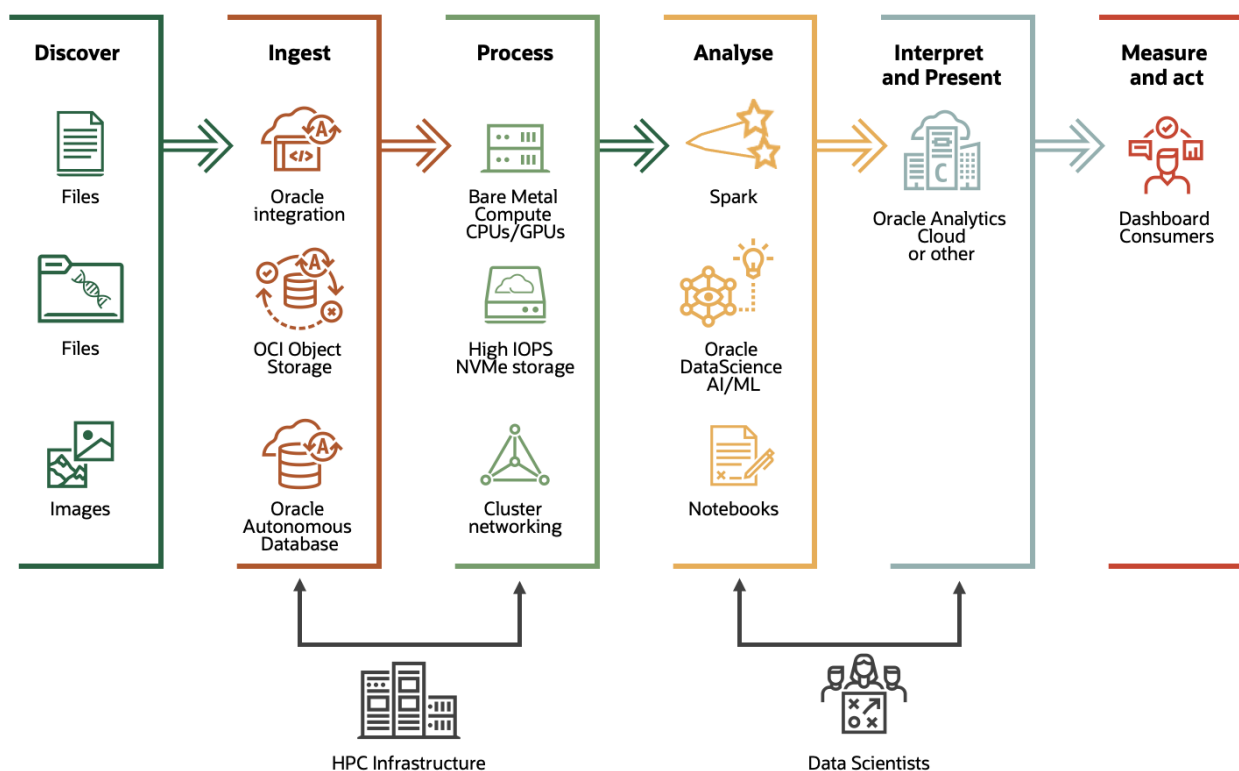
Oracle's Gen 2 Cloud enables organisations to run any workload at any time over an infrastructure that matches and surpasses the performance, control, and governance of institutional data centres while delivering the scale, elasticity, and cost savings of public clouds.

- High availability across multiple regions, availability domains, and fault domain configurations that are non-oversubscribed.
- High-performance with high-frequency cores, specialty-compute instances and 100 Gbps networking for remote direct memory access (RDMA). OCI's RDMA network allows customers to configure compute nodes into a high bandwidth ultra-low latency network that can go as low as 1.5 μ s.
- High scalability with autoscaling to adjust resources up and down automatically in response to changing demands.

Oracle Gen 2 Cloud offers the latest, high-end components, support for third-party and open-source technologies, unique support for hybrid and multi-cloud strategies, and an unwavering commitment to protect sensitive data. It's

a security-first architecture with workload isolation at all levels of networking, storage, and compute, with no over-provisioning of services at any point, giving customers uniformly high and predictable performance with service-level agreements for all workloads at any given time. This also gives Oracle a highly advantageous cloud cost model, where, simply put, faster is cheaper.

Integrated data platform architecture with HPC



Why HPC is better on Oracle than other clouds

HPC is the key enabler for innovation and delivering leading-edge products and services. However, access to HPC has not always been simple and cost effective. High cost and capital requirements act as a barrier to both small and large pharma organisations, to realise the possible, to evolve the next.

Oracle HPC sources of value

ORACLE DIFFERENTIATOR	DETAIL
Latest in compute hardware	<ul style="list-style-type: none"> Run your HPC workloads on next-generation hardware (NVIDIA, AMD, and Intel). Get on-premise levels of performance and control using dedicated bare metal instances.

	<ul style="list-style-type: none"> • Get better price-performance than with other cloud vendors. (E.g. Oracle is typically 44 percent less expensive than Amazon Web Services for Computational Fluid Dynamics (CFD) workloads for Ansys Fluent CFD workloads)
Scalable, independent instances, more than any storage	<ul style="list-style-type: none"> • Get 6.4 TB of local NVMe flash storage. • Get extreme, low-latency storage for shared-nothing architectures or fast, local scratch storage. • Leverage elastic block storage volumes for additional storage that can provide up to 32 TB each and up to 35,000 IOPS per volume, backed by performance service-level agreements. • Choose from wide set of parallel file systems that can be deployed in three clicks.
Specialised network	<ul style="list-style-type: none"> • Achieve 100 Gbps network throughput with latency under 1.5 microseconds with secure, dedicated RDMA over converged Ethernet (RoCE) v2. • Scale up to 20,000 cores in a single RDMA cluster with latency as low as 1.5 microsec. • Access compute clusters fast with non-oversubscribed flat network with dual 25 Gbps bandwidth. Easily move your existing network topology to the cloud with virtual cloud networks. • Leverage the only cloud with network performance service-level agreements.

Our growing collaboration with Oracle is fuelling incredible innovations across a wide range of industries and uses. By integrating NVIDIA's new A100 Tensor Core GPUs into its cloud service offerings, Oracle is giving innovators everywhere access to breakthrough computing performance to accelerate their most critical work in AI, machine learning, data analytics and high-performance computing."

Ian Buck

Vice President and General Manager of Accelerated Computing, NVIDIA

Conclusion

The pharmaceutical industry is facing unprecedented pressures. A core focus for organisations is to address R&D cost structures and improve discovery and development efficiency and effectiveness. At the heart of achieving this is the acquisition and analysis of data and its subsequent transformation into actionable insight. Oracle Cloud Infrastructure HPC is a key enabler to improving the economics of pharmaceutical R&D. It requires fewer prototypes, accelerates testing, and decreases time to market. The technology is callable on demand, suitable for any HPC workload, based on the most advanced compute, storage, networking, and software technologies, and allows pharma companies to pay for only what they use.

Moreover, Oracle Cloud Infrastructure HPC fits within a wider set of cloud-based digital platforms and can integrate any data sources into a comprehensive data platform that supports AI and machine learning to deliver business value. Data that had previously been locked in silos can now be released and given a voice to help drive better outcomes across the R&D value chain—from discovering data sources and analysing, transforming, and reining them to getting the analysis and insight to empower decision-making. As unlike first generation cloud vendors, Oracle Gen 2 Cloud has been architected for security, performance/price and comprehensive SLAs throughout, which is why organisations are now turning to Oracle.

The pharma industry now has the opportunity to add tremendous value and be at the heart of the simulated, digital patient journey. However, as with many other disrupted industries, the success of individual players will hinge on the speed at which they can transform themselves to meet the new market reality.

Why move HPC workloads to Oracle Cloud Infrastructure?

- Gain performance that matches and even exceeds on-premises deployments
- Complete simulations, renderings, and AI training fast with the highest-performing IaaS among public clouds
- Scale infrastructure up and down quickly, and pay only for the resources that you use
- Pay for compute-intensive workloads as predictable operational expenses, and avoid massive capital expenditures
- Focus on your simulations and renderings—not on keeping up with the latest hardware and software

Watch the video on YouTube, [Oracle Unlocks HPC](#).

Discover High Performance Computing on [Oracle Cloud Infrastructure](#).

Appendix: Examples of successful HPC projects with Oracle

Flinders University identifies candidate for Covid-19 vaccine

Australian researchers are testing a vaccine candidate against the SARS-CoV-2 coronavirus responsible for the COVID-19 pandemic. Supported with a one-year Oracle for Research grant, the research team is worked to accelerate vaccine discoveries with Oracle Cloud technology and vaccine technology developed by local company Vaxine Pty Ltd. They used computer models of the spike protein and its human receptor, ACE2, to identify how the virus was infecting human cells, and then were able to design a vaccine to block this process.



"The team has exploited the very latest technologies, including AI, advanced manufacturing, and Cloud computing to accelerate vaccine design, shaving years off normal development timeframes."⁴

Professor Petrovsky, Flinders University Professor and Research Director at Vaxine

Bristol, French National Centre for Scientific Research (CNRS) and Oracle join forces against tropical disease

Scientists from University of Bristol and the French National Centre for Scientific Research (CNRS) have identified a candidate synthetic vaccine against the tropical disease Chikungunya.



"We processed the large data sets obtained by the microscope on the cloud in a fraction of the time and at much lower cost than previously possible. We took a 90-day process and completed it in under five days with Oracle Cloud HPC."

Christopher Woods, EPSRC Research Software Engineer Fellowship

Altair runs complex simulations on Oracle Cloud Infrastructure

Altair HyperWorks Unlimited Virtual Appliance is a fully managed engineering service that provides modelling and visualization software, solvers, and postprocessing tools—all on Oracle Cloud Infrastructure. They have achieved 25 percent better price-performance on Oracle Cloud Infrastructure versus other cloud providers.



"We went looking for the best price-performance, and we found that in Oracle Cloud Infrastructure."

Sam Mahalingam, Chief Technical Officer for Enterprise Solutions, Altair Engineering

⁴ <https://news.flinders.edu.au/blog/2020/04/03/flinders-targets-covid-19-vaccine/>

Gridmarkets run molecular simulations with Brigham Young University, Texas A&M University

Researchers use X-ray diffraction and 3D molecular-modelling software to build a crystal structure of the virus that causes COVID-19. Using Oracle HPC, the animation rendering platform can render complex molecular models in less than 24 hours.



"We don't own or maintain any hardware, and we're paying 70 percent less to spin up an instance on Oracle Cloud infrastructure than we did running workloads on Amazon Web Services or Google Cloud,"

said GridMarkets Cofounder Mark Ross.

Manchester Metropolitan University and NHS use AI to identify diabetic foot wounds

Manchester-based app Footsnaps AI, supported by Oracle for Research, can identify diabetic foot ulcers and associated pathologies and provide feedback within 20 seconds using Oracle Cloud Infrastructure. With an amputation rate 36 percent above the UK national average, Footsnaps AI used deep learning to provide near real-time medical feedback as well as reduce foot-ulcer-related visits by an expected 50 percent.



"Understanding the treatment of ulceration and whether these wounds are getting better or worse is essentially pattern recognition. Further, the real breakthrough will come if we - health professionals and patients - can identify these wounds much earlier and therefore initiate much more timely treatment. This is where artificial intelligence is potentially a game changer,"

says Naseer Ahmad, Consultant Vascular Surgeon at Manchester University NHS Foundation Trust.

Elem Biotech creates virtual humans to aid clinical trials

ELEM generates 3D models of human organs from patient scans to provide an almost unlimited virtual clinical trials platform. Thanks to the simulation engine and the cloud database, it is possible, for example, to simulate obstructive lung diseases or to replicate the functioning of pacemakers, valve replacements, stents, anti-arrhythmic drugs, and treatments for asthma or drug pumps.



"Our virtual humans, which reduce animal and human testing, as well as product cost and time to market, are created in the Oracle Cloud infrastructure, where medical device manufacturers, pharmaceutical companies, and researchers can analyze their products and optimize treatments to better meet patient needs,"

said Christopher Morton, CEO of ELEM Biotech.

Gromacs simulates the movements of atoms in biomolecules



Gromacs is a molecular dynamics software that simulates the movements of atoms in biomolecules under a predefined set of conditions. It is used to identify the behaviour of these biomolecules when exposed to changes in temperature, pressure, and other inputs that mimic the actual conditions encountered in a living organism. Gromacs can be used to establish patterns in protein folding, protein-ligand binding, and cell-membrane transport, making it a very useful application for drug research and discovery.

Oracle Cloud Infrastructure gets behind world's fastest supercomputer



RIKEN is the owner of the world's fastest HPC supercomputer known as Fugaku. RIKEN has chosen Oracle Cloud Infrastructure as the public cloud provider for its elastic HPC storage and to enable universities and research organizations to connect securely and cost-effectively through the Science Information Network (SINET). Oracle was chosen because of its superior performance, enterprise-grade security, and elastic storage resources as part of the ongoing initiative to promote wider use of the supercomputer.

University of Oxford combines telecoms and healthcare data to model pandemic



University of Oxford turned to Oracle for Research and the power of Oracle Cloud Infrastructure Data Science to model the UK's COVID-19 exit strategy and economic recovery. The work brings together mobile phones, social media, and demographics into single data platform. The result is the ability to understand population movement as an indicator of virus transmission at a local level with up to two metres of accuracy.

Using this big data at different geographical levels, the team can predict capacity pressures on hospitals based on population movement in the local communities that they serve, predict where it may be possible to ease social distancing measures at the regional and local levels, and monitor which areas of the country are re-opening for business and which are not.

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