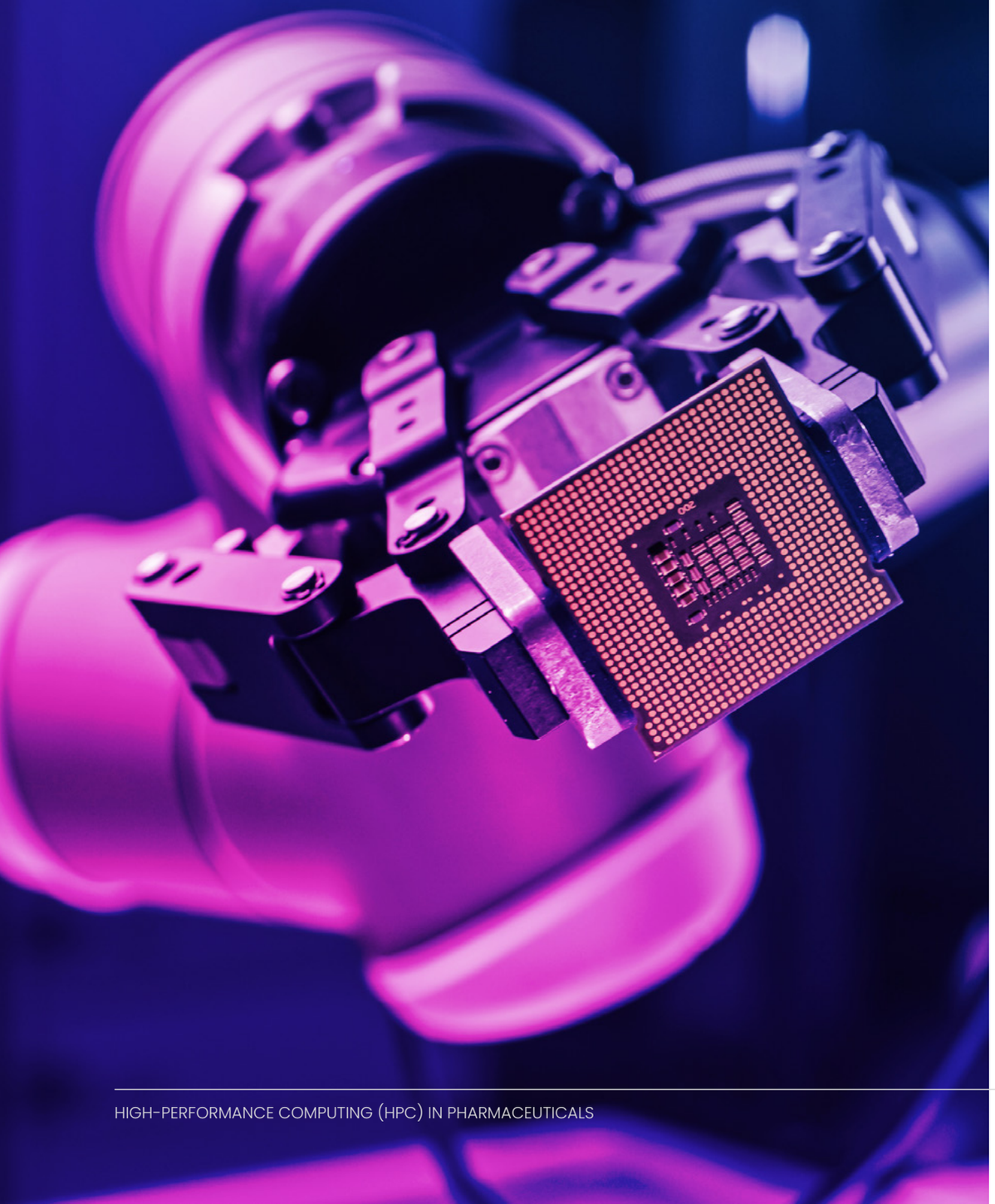
HIGH-PERFORMANCE COMPUTING (HPC) IN PHARMACEUTICALS

THE OCF AND NVIDIA EXPLAINER GUIDE



HPC: ACCELERATING MEDICINE INNOVATION AT SCALE

Drug discovery and development is a complex and time-consuming process. Speeding up the route to market, for new medicines and new applications for existing drugs, is critical. Not just for business success but for saving lives.

Faster processes allow pharmaceutical companies to capitalise on the small window of profitable opportunity that follows immediately after a drug is launched. And it allows patients to benefit sooner from the transformative benefits of new and revolutionary treatments and drug development techniques.

As the volumes of data created by the pharmaceuticals industry continues to grow exponentially, HPC can provide the raw power needed to process this data and uncover the insights that speed innovation and drive successful operations. It can also support the careful storage and management of sensitive data created in the process of producing and trialling drugs.

Pharmaceutical companies need this clarity of data to quickly identify ‘dead end drugs’, so they can prevent waste and ensure resources are invested into viable alternatives. This is especially important to charities working with limited budgets – where innovation must be delivered at the lowest possible cost.

Fully understanding the benefits of HPC, and how to embrace them, is a common concern for pharmaceutical companies.

This guide highlights the value and real-world use cases of HPC, exploring challenges and showing how OCF and NVIDIA offer the solutions needed to help businesses reap the full insights from their data.

THE BENEFITS OF HPC

HPC accelerates drug discovery by simulating huge workloads to create accurate iterations in minutes rather than days or even weeks – maximising the time available for drug discovery.

HPC consolidates compute power into a centralised resource, helping to optimise resource measurement, management and allocation, in a more dynamic and less wasteful way.

HPC attracts and retains the best talent by providing an environment where researchers are empowered and their work is supported by the best possible technology.

It's predicted we'll generate **463 exabytes of data per day** by 2025.[1]

HPC performs **quadrillions of calculations** per second.[2]

Global research shows that **97% of companies** that have adopted HPC platforms say they won't survive without one. [3]

HOW ARE INDUSTRY LEADERS USING HPC?

FAST TRACKING DISCOVERY AND DEVELOPMENT WITH GPU-POWERED HPC

GPUs (Graphics Processing Units) are emerging as a powerful tool for supporting HPC in drug discovery and development – speeding up intensive computer-related tasks such as molecular docking or machine learning algorithms. By utilising GPUs' processing power, developers can quickly identify promising drugs and accelerate time to market.

The NVIDIA A100 Tensor Core GPU is a popular choice for drugs discovery with small workstation-sized systems, while the NVIDIA H100 Tensor Core GPU and the NVIDIA H200 Tensor Core GPU are ideal for large-scale drug discovery.

HOW ARE INDUSTRY LEADERS USING HPC?

POWERING RESEARCH AT THE WELLCOME TRUST

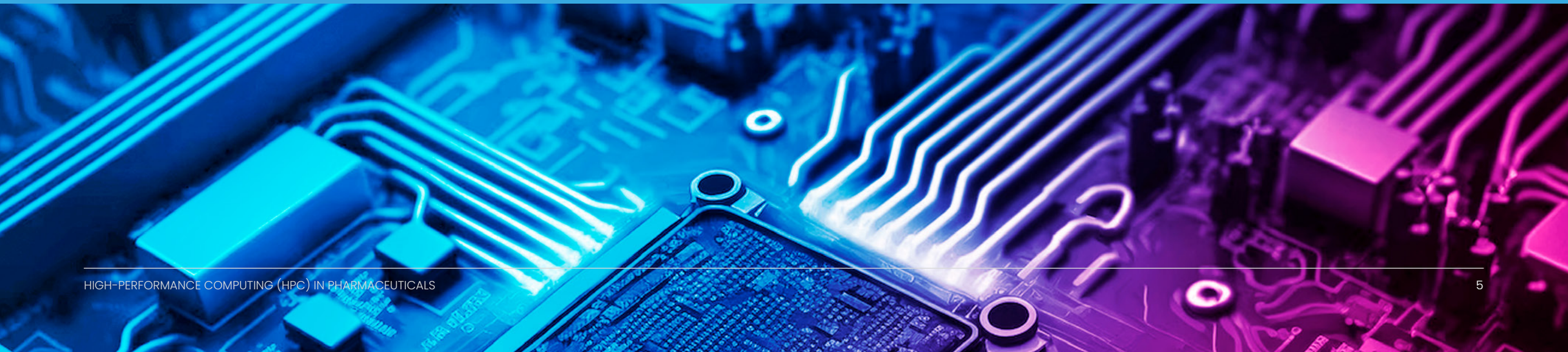
The Wellcome Trust Centre for Human Genetics (WTCHG) is a research institute based at the University of Oxford. It's an international leader in genomics, statistical genetics and structural biology, and it collaborates with research teams from across the world on a number of large-scale studies.

WTCHG sequences around 500 genomes a year and stores approximately 20,000 (over half a petabyte) on high-speed disk for analysis – as a result it needed to increase its compute power to support its research.

OCF worked in partnership with WTCHG to design a high-spec cluster and storage system. By understanding the characteristics of key genetics applications and optimising how it maps onto the new cluster's architecture, WTCHG dramatically improved the efficiency of its analysis from months to weeks.

The new cluster has also helped support WTCHG's Division of Structural Biology and produced some of the world's highest resolution electron microscopy reconstruction.

> "Research is driving our adoption of HPC. Compared to this time last year, our researchers can put through five times more work on a machine with the same energy footprint."
>
> Dr Esnouf, Head of the Research Computing Core at WTCHG



WHY ARE PHARMACEUTICAL COMPANIES HESITANT TO EMBRACE HPC?

LACK OF SKILLS

Pharmaceutical companies – particularly startups with limited resource and budget – face a significant skills gap in delivering HPC. The shortage is especially acute when delivering at scale.

TALENT RETENTION

Without the right tools, retaining skilled researchers can be a challenge – many will move to competitors if they aren't provided with the most current and advanced technology.

CLOUD COSTS

Given the industry's huge data volumes, the cloud becomes expensive when migrating data.

UNCLEAR ROI

Understanding the ROI achievable with HPC can also be a challenge for many.

OPEN-SOURCE OBSTACLES

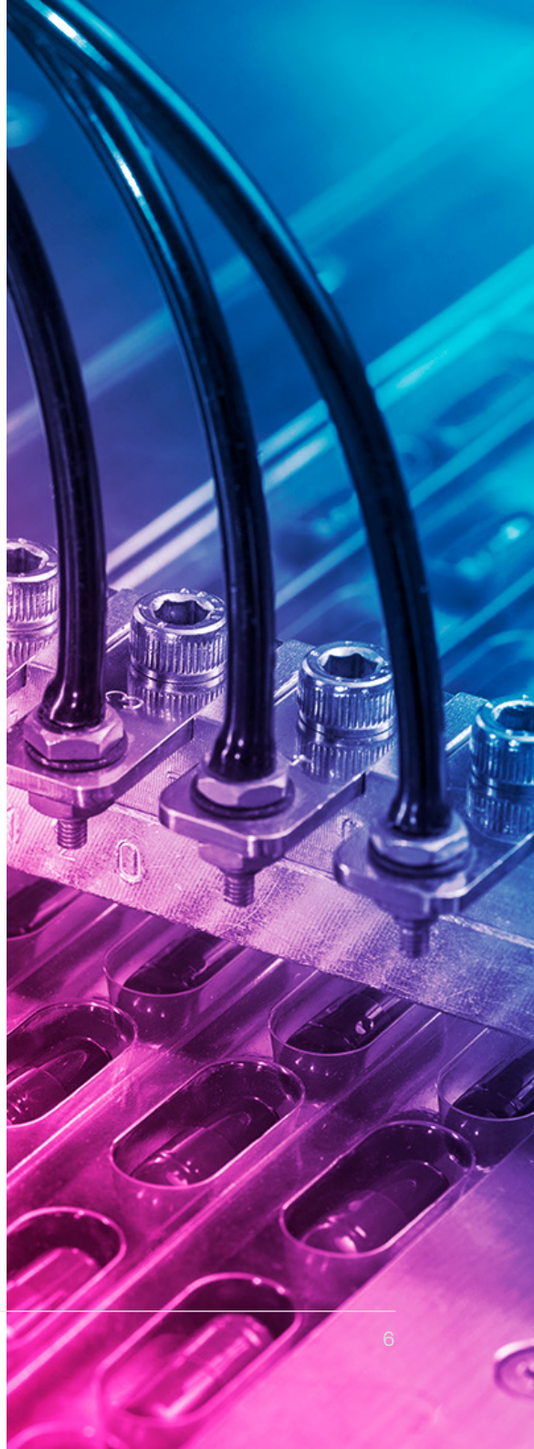
Managing and working with open-source software has become complicated due to lack of production-ready workflows.

OCF IN ACTION

OCF can help pharmaceutical businesses understand ROI by benchmarking how quickly systems can work and identifying the time and resource that can be saved.

75% of IT executives say talent shortages are their biggest risk factor in deploying technology.[4]

42% of digital leaders are struggling to find people with data and analytics skills in the UK.[5]

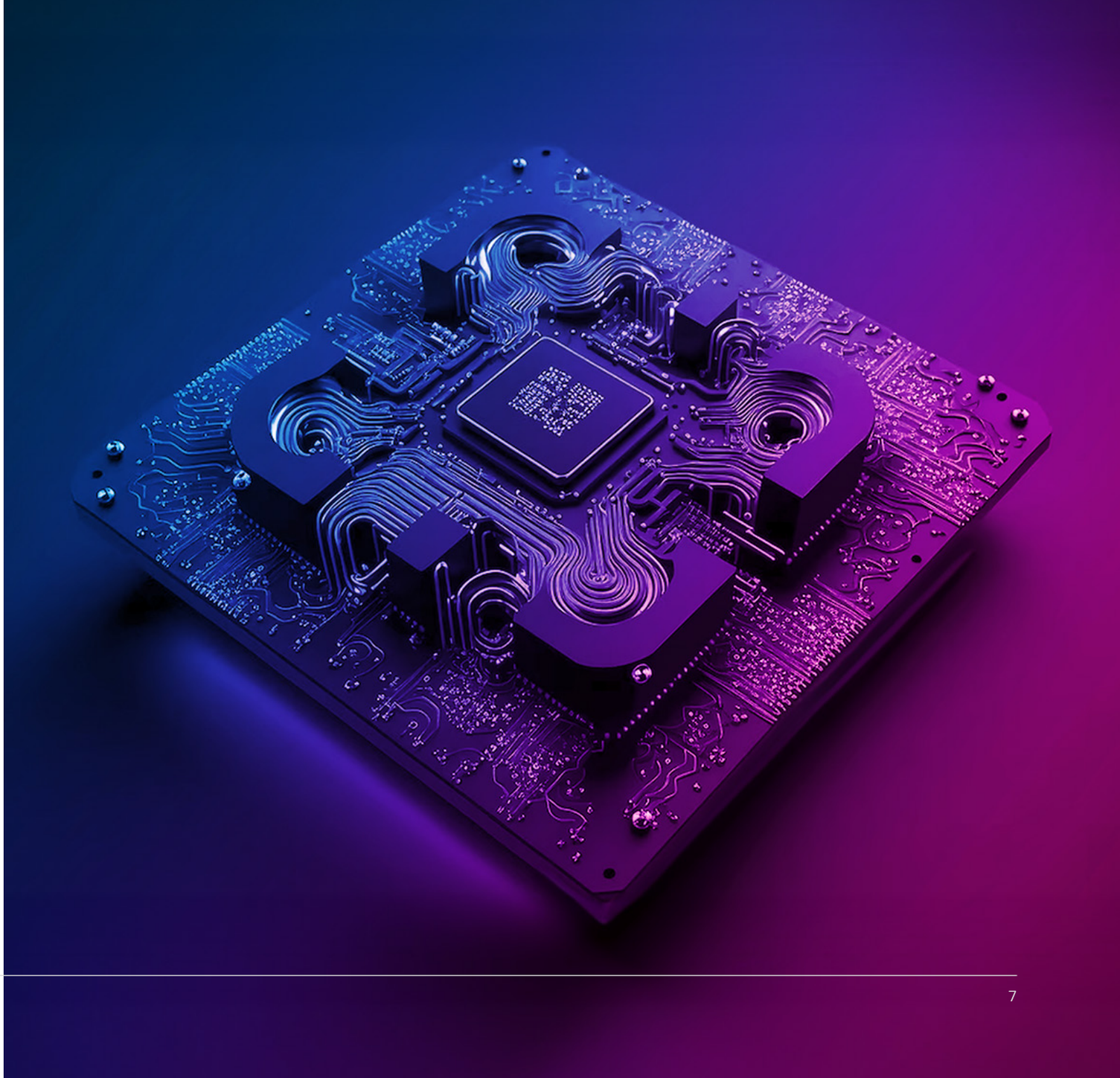


UNLOCK THE POWER OF HPC WITH OCF AND NVIDIA

OCF and NVIDIA empower pharmaceutical companies to unlock the potential of a secure and powerful HPC solution to meet existing and future performance demands.

With HPC from OCF and NVIDIA, businesses can free up teams to focus on their goals – whether that's working on other IT projects or utilising the new compute to accelerate research and development.

For every **$1 invested** in HPC, Life Sciences generate **$160 in revenue** with **$41 of that being profit**.[6]

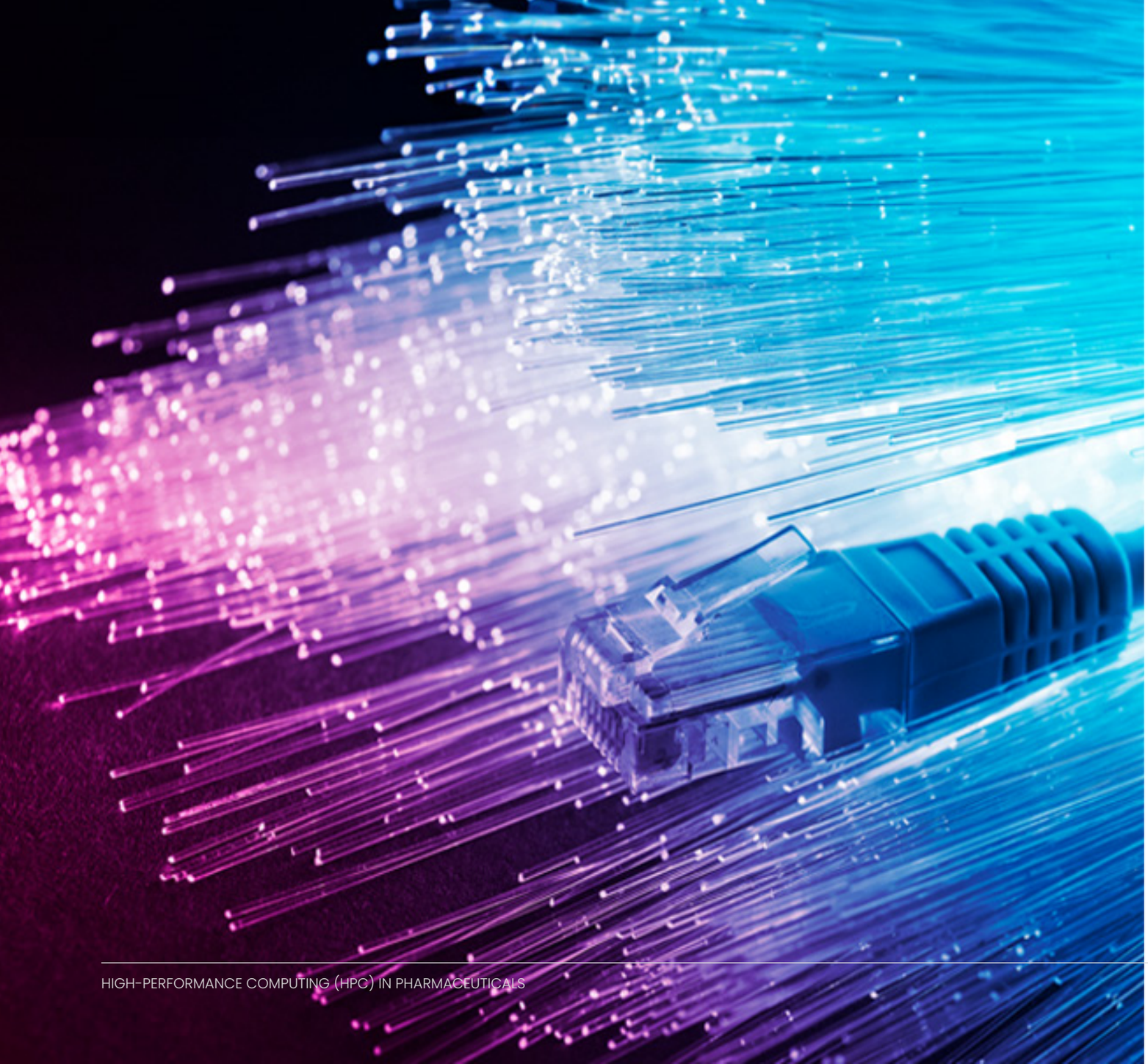


OCF's team is comprised of seasoned industry experts, with many having over 20 years of experience with HPC – ensuring OCF's team can work with first-time buyers or more experienced customers.

As an Elite NVIDIA partner, OCF offers customers a true end-to-end experience, working from initial consultancy through to design and managed services.

OCF's in-house technical architects develop solutions from tried-and-tested building blocks – ensuring best practices are at the heart of every solution – before optimising and tailoring them to suit specific customer needs. And OCF's experts provide ongoing support to adapt HPC solutions as a customer's business needs and challenges change, futureproofing investments.

OCF offers a managed service to alleviate the technical and skills-shortage challenges of day-to-day administration for HPC clusters. In addition, OCF offers training sessions to ensure every key worker is equipped with the HPC knowledge they need.



NVIDIA

NVIDIA's high-performance in-network technology enables large amounts of data to be transmitted quickly and efficiently – delivering maximum output from HPC infrastructure.

With the choice of InfiniBand or Ethernet, NVIDIA provides a comprehensive, end-to-end, high-performance solution. It's also the world's only fully offloadable, In-Network Computing platform.

NVIDIA networking products are designed to allow businesses to start small and scale when required – ensuring growth occurs when appropriate and without wastage. And as your computing demands grow, NVIDIA gives you the flexibility and scalability to manage complex workloads and extreme-sized data sets without compromising on speed.

NVIDIA also offers extensive support when using in-house code on its GPUs.

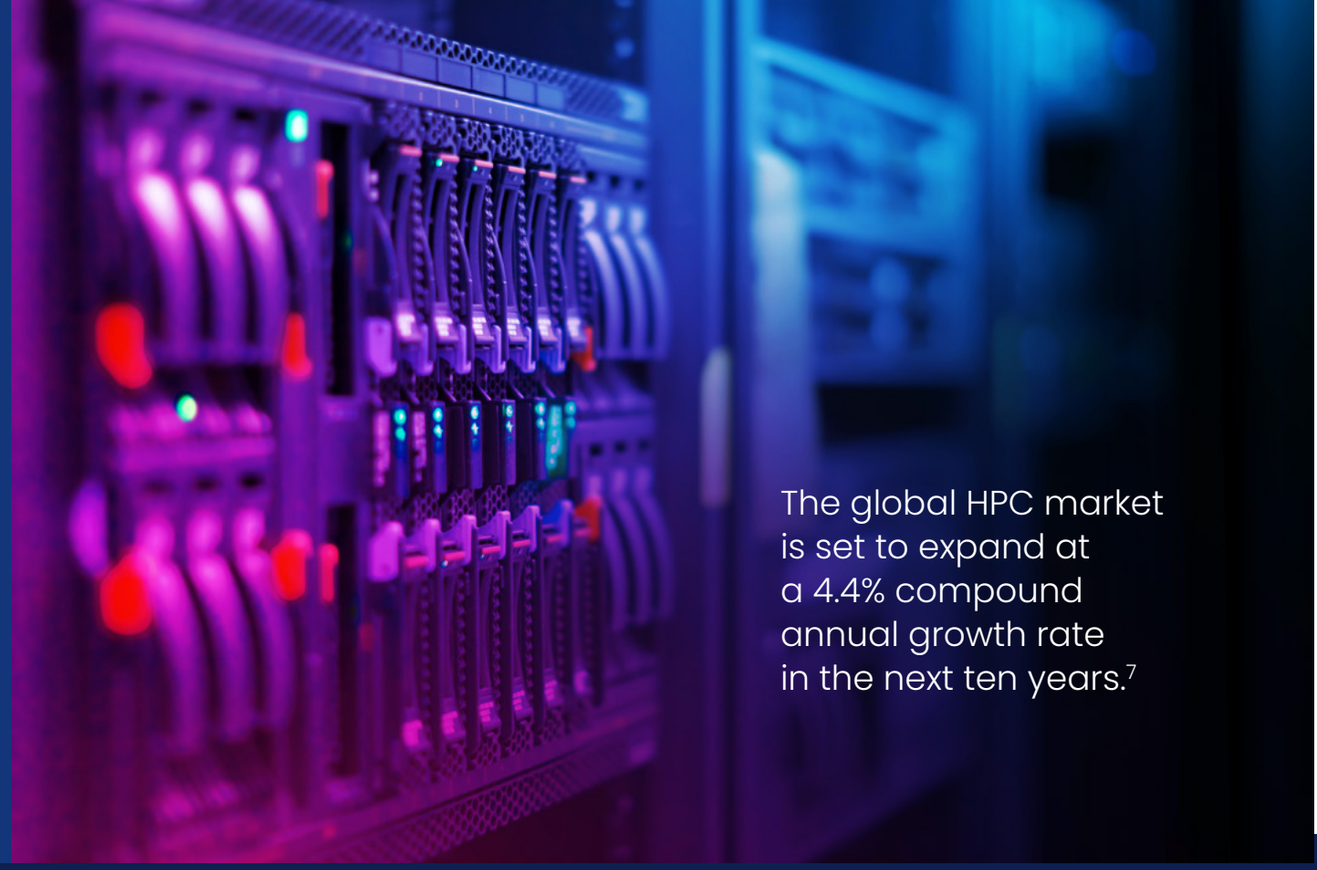
END-TO-END HPC SUCCESS STARTS WITH OCF AND NVIDIA

OCF and NVIDIA are the key to unlocking the full benefits of every HPC solution. OCF combines decades of technical expertise with trusted partnerships to develop and deliver an industry-leading, NVIDIA-powered HPC solution.

OCF works collaboratively with NVIDIA and other independent software vendors to understand existing and emerging challenges facing the pharmaceuticals sector.

OCF's experts are problem solvers with the technical expertise needed to identify bottlenecks in your systems and the ideal solutions to solve them – examining:

- Your current IT usage and what needs to be updated, replaced, or optimised
- Your current in-use applications and whether they are scalable, optimisable, and compatible with HPC



The global HPC market is set to expand at a 4.4% compound annual growth rate in the next ten years.[7]

TECHNICAL PRE-SALES CONSULTANTS

Experts in solution architecture design and able to evolve your solution with changing demands.

BUSINESS DEVELOPMENT MANAGERS

Relationship builders with deep technical expertise, able to understand and act on your short and long-term business demands.

HPC TECHNICAL CONSULTANTS

A team of highly skilled consultants with leading expertise across NVIDIA HPC solutions and its wider portfolio.

IT PROJECT MANAGERS

PRINCE2 certified and highly experienced in delivering NVIDIA HPC solutions using proven methodologies.

OCF'S END-TO-END PROCESS

RESEARCH

OCF's experts explore your business' short and long-term compute needs and challenges.

DESIGN

The OCF team explores different HPC options to suit your defined business requirements, budget constraints, and timeline goals.

PRESENT

OCF presents you with everything our team has learned, including any insights and recommendations, before we agree on an approach.

DOCUMENT

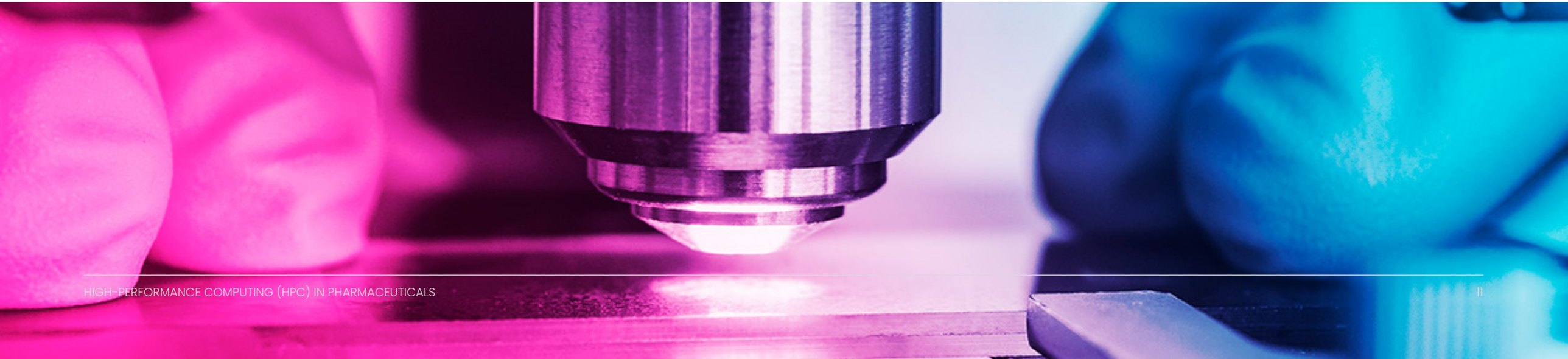
You receive a detailed document outlining the approach and plan for implementation.

IMPLEMENT

OCF's technical experts work to deliver the solution.

REVIEW

OCF's team measures success to develop future optimisation and strategies.



CONTACT OCF FOR NVIDIA TODAY

With HPC from OCF and NVIDIA your pharmaceutical business can discover, develop and bring medicines to market at speed. With the best technology in place, you'll attract and retain the best talent – and they'll be empowered to deliver life-saving innovations faster with high-impact data processing behind them.

At OCF, we examine your business' needs, challenges, and priorities, and develop a scalable HPC solution that's unique to you. Our years of experience mean we can offer ongoing support as your business grows – helping to futureproof your system and deliver continuous optimisations.

Accelerate your discovery with OCF and NVIDIA.
Get in touch to find out more.

Contact now

Sources

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2 Tech Target, 2021
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4 Gartner, 2021
5 Computer Weekly, 2022
6 HPCwire, 2020
7 Global News Wire, 2023